19 BUNDESREPUBLIK DEUTSCHLAND

- _® DE 102 59 786 A 1

Offenlegungsschrift

(5) Int. Cl.⁷: C 12 N 9/12 A 61 K 31/427



DEUTSCHES PATENT- UND MARKENAMT

- (21) Aktenzeichen:
- 102 59 786.3 ② Anmeldetag:
- 19. 12. 2002 (3) Offenlegungstag: 17. 7.2003
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(3) Unionspriorität:

341988

19. 12. 2001 US

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Prüfungsantrag gem. § 44 PatG ist gestellt

- (6) Kristalle der Glukokinase und Verfahren zu ihrer Züchtung
- Kristalline Formen von Säuger-Glucokinase von ausreichender Größe und Qualität und Strukturdaten mit Hilfe von Röntgenkristallographie zu erhalten, werden dargestellt. Verfahren zur Züchtung solcher Kristalline sind ebenfalls offenbart.

Beschreibung

[0001] Die Erfindung betrifft kristalline Formen der Glucokinase von ausreichender Größe und Qualität um Strukturdaten mittels Röntgenkristallographie zu erhalten und Verfahren zum Züchten solcher Kristalle.

[0002] Glucokinase (GK) ist eine von vier Hexokinasen, die in S\u00e4ugern gefunden worden sind [Colowick, S.P., in The Enzymes, Bd. 9 (P. Boyer, Hrsg.) Academic Press, New York, NY, S. 1-48, 1973]. Die Hexokinasen katalysieren den ersten Schritt des Glucosemetabolismus, d. h. die Umwandlung von Glucose zu Glucose-6-Phosphat. Glucokinase hat eine begrenzte zelluläre Verteilung und wird vornehmlich in pankreatischen B-Zellen oder Parenchymzellen der Leber gefunden, Zusätzlich ist GK ein Geschwindigkeits-kontrollierendes Enzym des Glucosemetabolismus in diesen beiden Zelltvpen, von denen bekannt ist, dass sie eine entscheidende Rolle bei der Glucose-Homöostase des ganzen Körpers spielen [Chipkin, S.R., Kelly, K.L., und Ruderman, N.B. in Joslin's Diabetes (C.R. Khan und G.C. Wier, Hrsg.), Lea und Febiger, Philadelphia, PA, S. 97-115, 1994]. Die Glucosekonzentration bei der die GK eine halbmaximale Aktivität zeigt ist annähernd 8 mM. Die anderen drei Hexokinasen sind bei deutlich geringeren Konzentrationen (<1 mM) gesättigt. Daher steigt der Glucosefluss durch den GK-Stoffwechselweg an, wenn sich die Glucosekonzentration im Blut nach einer kohlenhydrathaltigen Mahlzeit von Fasten(5 mM)- zu Postprandial(~10-15 mM)-Spiegeln erhöht [Printz, R.G., Magnuson, M.A., und Granner, D.K. in Ann. Rev. Nutrifion Bd. 13 (R.E. Olson, D.M. Bier, und D.B. McCormick, Hrsg.), Annual Review, Inc., Palo Alto, CA, S. 463-496, 1993]. Diese Erkenntnisse trugen vor über einem Jahrzehnt zur Hypothese bei, dass GK als Glucosesensor in β-Zellen und Hepatocyten fungiert (Meglasson, M.D. und Matschinsky, F.M. Amer. J. Physiol. 246, E1-E13, 1984). In den letzten Jahren haben Untersuchungen an transgenen Tieren bestätigt, dass GK tatsächlich eine entscheidende Rolle bei der Glucose-Homöostase des ganzen Körpers spielt. Tiere, die keine GK exprimieren sterben innerhalb weniger Tage nach der Geburt mit schwerer Diabetes, während Tiere, die GK überexprimieren eine verbesserte Glucosetoleranz aufweisen (Grupe, A., Hultgren, B., Ryan, A. et al., Cell 83, 69-78, 1995; Ferrie, T., Riu, E., Bosch, F. et al., FASEB J., 10, 1213–1218, 1996). Werden β-Zellen in erhöhtem Maße Glucose ausgesetzt, ist dies über GK-Kopplung in den β-Zellen mit einer erhöhten Insulinausscheidung verbunden. Werden Hepatocyten in erhöhtem 25 Maße Glucose ausgesetzt, ist dies über GK-Kopplung in den Hepatocyten mit erhöhter Glykogenablagerung und viel-

leicht reduzierter Glucoseproduktion verbunden.

[9003] Die Erkenntris, dasse Typ II-Diabetes, das bei jungen Erwachsenen ausbricht (MODY-2, "maurity-onset diabetes of the young") durch Mutationen im GK-Gen verursacht wird, die zum Verlust der Funktion führen, deutet daraufhin, dass GK auch als Glucosesensor im Menschen fungiert (Liang, Y., Kesavan, P., Wang, L. et al., Biochenn. J. 309, 30 167–173, 1995). Ein zusätzlicher Beweis, der die wichtige Gelle von GK bei der Regulierung des Glucose-Metabolismus im Menschen stützt, wird durch die Identifizierung von Patienten geliefert, die eine mutierte Form von GK mit erhöhter Enzymaktivität exprimieren. Diese Patienten zeigen eine Faster-Hypergly-Känike verbunden mit einem unangemessen erhöhten Plasma-Insulinspiegel (Glaser, B., Kesavan, P., Heyman, M. et al., New England J. Med. 338, 226–230, 1998). Obwohl bei einem Großeit der Patienten mit Typ II-Diastes keine Mutationen des GK Gens gefunden werken, sind verbindungen die GK aktivieren und dadurch die Empfindlichkeit des GK-Sensorsystem erhöhen immer noch für die

35 Verbindungen die GK aktivieren und dadurch die Empfindlichkeit des GK-Sensorsystem erhöhen immer noch für die Behandlung der hyperglyklminschen Charakteristiken aller Typ II-Diabetes nützlich. Glucokinase-Aktivatoren steigern den Fluss des Glucose-Metabolismus in F-Zellen und Hepatocyten, der mit einer erhöhten Insulinausscheidung verbunden ist. Solche Mittel w\u00e4ren f\u00fcr die Behandlung von Typ II-Diabetes n\u00fctzlich sitzlich.
[0004] Es wird oft versucht die Kristallstruktur solcher Proteine zu bestimmen, insbesondere bei Anstrengungen den

40 Mechanismus aufzuklären, der der Kinase-Aktivierung unterliegt. Die Kristallstrukturen verschiedener Hexokinasen sind veröffentlicht worden Siche z. B. A.E. Aleshin, C. Zeng, G.P. Bourenkov, H.D. Barunik, H.J. Fromma & R.B. Honzatko "The mechanism of regulation of hexokinase: new insights from the crystal structure of recombinant human brain hexokinase complexed with glucoses and glucose-2-phosphate "Structure dietermination and refinement at 3.5 Å resultion" J. Mol.Biol. 140, 183–209 (1978); und S. Ito, S. Fushinobu, I. Yoshioka, S. Koga, H. Matsuzawa & T. Wakagi "Structural Basis for the ADD-Specificity of a Novel Glucokinase from a Hyperthermophilic Archaeon" Structure?

Structural Basis for the ADP-Specinicity of a Novel viluodomase from a Hyperthermopmilic Archaeors "structure y, 205–214 (2011). Thoiz disease flerichte versuchten Forscher, die wussten wie man Krstalle der betreffenden Hexokinssen chällt, erfolglos Kristalle von jeder Säuger-Glucokinsas zu erhalten.

[0005] Die Anmelder haben Verfahrensamvestungen gefunden, welche die Kristallisation von Säuger-Glucokinsse mit

oder ohne einen gebundenen allosterischen Liganden ermöglichen. Die Kristallstruktur wurde mit Hilfe von Röntgenkristallographie bei einer Auflösung von 2.7 Å gelös. Siehe Fig. 3 und 4. Daher betrifft die Erfindung eine kristalline Form der Glucokinase und eine kristalline Form eines Komplexes der Glucokinase mit einem allosterischen Liganden. Die Erfindung betrifft ferner ein Verfahren zur Brzeugung von Glucokinasekristallen mit oder ohne einen gebundenen allosterischen Lisanden.

55 [0006] Fig. 1 zeigt Glucokinase-Co-Kristalle mit P6(5)22-Symmetric.

[0007] Fig. 2 zeigt die Aminosäuresequenz einer exprimierten Glucokinase, die zur Kristallisation verwendet wurde.
 [0008] Fig. 3 zeigt ein Bänderdiagramm der Struktur von Glucokinase, das die α-Helices und die β-Faltblätter zeigt.

[0009] Fig. 4 zeigt die Atomstrukturkoordinaten der Glucokinase gebunden an 3-Cyklopentyl-2-pyridin-4-yl-N-thia-zol-2-yl-propionamid.

60 [0010] Die vorliegende Erfindung betrifft kristalline Formen von Säuger-Glucokinase mit oder ohne an der allosterischen Stelle gebundenem Liganden, wobei die Kristalle von ausreichender Qualität und Größe sind um die dreidimensionale Röntgen-Beugungs-Struktur zu einer Auflösung von etwa 2,0 Å bis etwa 3,5 Å zu bestimmen. Die Erfindung betrifft auch Verfahren zur Herstellung und Kristallisstion der Glucokinase. Die kristallinen Formen der Glucokinase sowie die von ihren Kristallstrukturen abgeleiteten Informationen können verwendet werden um die Glucokinase-Aktivität zu analysieren und zu modiffizieren, sowie um Verbindungen zu identifizieren, die mit der allosterischen Stelle in Wechsel-

[0011] Die Kristalle der Erfindung schließen Apo-Kristalle und Co-Kristalle ein. Die Apo-Kristalle der Erfindung umfassen normalerweise im Wesentlichen reine Glucokinase. Die Co-Kristalle umfassen normalerweise im Wesentlichen

reine Glucokinase mit einem an der allosterischen Stelle gebundenen Liganden.

[0012] Es ist so zu verstehen, dass die kristallinen Glucokinasen der Erfindung nicht auf natürlich vorkommende oder natür Glucokinasen begenzu sind. Tauskhicht schließen die Kristalle der Erfindung auch Mutanten der nativen Glucokinasen ein. Mutanten der nativen Glucokinasen ein. Mutanten der nativen Glucokinasen werden erhalten durch Austausch von mindestens einem Aminosäurerest in einer nativen Glucokinase-Domiñne durch einen unterschiedlichen Aminosäurerest, oder durch Hinzuffigen oder Deletieren von Aminosäureresten innerhalb des nativen Polyperpids oder am N- oder C-Terminus des nativen Polyperpids oder am N- oder G-Terminus des nativen Polyperpids, und haben im Wesentlichen die gleiche dreidimensionale Struktur wie die native Glucokinase von der die Mutante abseluiet ist.

[0013] Unter "hat im wesentlichen die gleiche dreidinensionale Struktur" ist zu verstehen, dass man einen Satz von Atomstrukturkoordinaten eines Apo- oder Co-Kristalls hat, deren Standardabweichnung weniger als oder gleich etwa 2Å ist, wenn sie mit den Atomstrukturkoordinaten der nativen Glucokinase von der die Mutante abgeleiret ist, überlagert werden und wenn mindestens etwa 50% bis etwa 100% der α-Kohlenstoffatome der nativen Glucokinase bei der Überlagerung einesehlossen sind.

[0014] In einigen Fällen, um z. B. die Reinigung des Polypeptids usw. zu unterstützen, kann es besonders vorteilhaft oder günstig sein, Aninosäurersete einer nativen Giucokinase-Domäne zu erseitzen, zu entfernen und/oder hinzuzufügen 19 um passende Clonierungsstellen in der eDNA bereitzustellen, die für das Polypeptid codiert. Solche Substitutionen, Deletionen und/oder Additionen, welche die dreidimensionale Struktur der nativen Glucokinase im Wesentlichen nicht verändern sind für den Fachman offensichtlich.

19015] Es solle angemerkt werden, dass die hier in Erwägung gezogenen Mutanen keiten Glucokinase-Aktivität der gen midseen. Täustehlich werden Aminosäure-Substitutionen, Activitätionen oder-Tolentonen, die die Kinase-Aktivität der Glucokinase besintrichtigen, die sehe fisch deriedimensionale Struktur der Domäne nicht signifikant indern, bei der Erindung speziell in Betracht gezogen. Solche kristallien obleyen bei deriedimensionale Struktur der Domäne nicht signifikant indern, bei der Erindung speziell in Betracht gezogen. Solche kristallien obleyen der die davon erhaltenen Atomstrukturkonfibrachten können verwendet werden um Verbindungen zu identifikzieren, die an die native Domäne binden. Diese Verbindungen Können die Aktivität doer die native Domäne besinflussen.

[9016] Die abgeleiteten Kristalle der Erindung umfassen im Allgemeinen ein kristallines Glucokinasse-Polypoptid in 25 kovalenter Bindung mit einem oder einer mehrene Schwermetallationen. Das Polypoptid kann einer nativen oder einer musteiren Glucokinase entsprechen. Schwermetallatione, die nitztlich sind um abgeleitete Kristalle bereitzustellen, schließen beispielnat und nicht begrenzen Gold und Quecksilber ein, Alternativ können abgeleitete Kristalle aus Proteinen erzeugt werden, die Schwermetallatome in einer oder mehreren Aminosäuren eingebaut haben, uvie bei Selen-Methionis-Substitutionen für Methionia.

[0017] Die Co-Kristalle der Erfindung umfassen im Allgemeinen ein kristallines Glucokinase-Polypeptid in Verbindung mit einer oder mehreren Verbindungen an der allosterischen Stelle des Polypeptids. Die Bindung kann kovalent oder nicht kovalent sein.

[0018] Die hierin beschriebenen nativen und mutierten Glucokinasse-Polypeptide können aus natürlichen Quellen isolient werden oder über Verfahren, die dem Pachmann der Molekularbiologie gut bekannt sind, hergestellt werden. Die 15 Expressionsvektoren, die verwendet werden sollen, können eine codierende Sequenz des nativen oder mutierten Glucokinasse-Polypeptids und geeignete transkriptionselle und/doet translatorische Kontrollsignale enthalten. Diese Verfahren schließen in vitro-DNA-Rekombinations-Verfahren, synthetische Verfahren und in vivo-Rekombination/genetische Rekombination in: Siehe z. B. das in Maniatisct a. I, 1989, Molecular Cloning: A. Laboratory Manual, Cold Spring Harbor Laboratory, NY; and Ausubel et. al., 1989, O'urrent Protocols in Molecular Biology, Green Publishing Associates and Willey Intersclence, NY beschriebene Verfahren.

[0019] Eine Vielzahl von Wirt-Expressionsvektor-Systemen können verwendet werden, um die Glucokinase codierende Sequenz zu exprimieren. Diese schließen ein ohne darauf begrenzt zu sein: Mikroorganismen wie mit rekombinanter Bakteriophagen-DNA transformierte Bakterien; Plasmid-DNA- oder Cosmid-DNA-Expressionsvektoren, die die Glucokinase codierende Sequenz enthalten; Hefe, transformiert mit rekombinanten Hefe-Expressionsvektoren, die die Glucokinase codierende Sequenz enthalten; Insektenzellsysteme, infiziert mit rekombinanten Virus-Expressionsvektoren (z. B. Baculovirus), die die Glucokinase codierende Sequenz enthalten; Pflanzenzellsysteme, infiziert mit rekombinanten Virus-Expressionsvektoren (z. B. Blumenkohl-Mosaikvirus, CaMV; Tabak-Mosaikvirus, TMV) oder transformiert mit rekombinanten Plasmid-Expressionsvektoren (z. B. Ti-Plasmid), die die Glucokinase codierende Sequenz enthalten; oder Tierzellsysteme. Die Expressionselemente dieser Systeme variieren in ihrer Stärke und Spezifitäten. Abhängig vom verwendeten Wirt/Vektor-System können beliebige einer Reihe von geeigneten Transkriptions- und Translationselementen verwendet werden, einschließlich konstitutive und induzierbare Promotoren wie pL des Bakteriophagen u. plac, ptrp, ptac (ptrp-lac-Hybrid-Prormotor) und ähnliche. Bei der Glonierung in Insekten-Zellsystemen können Promotoren, wie der Baculovirus-Polyhedrin-Promotor, verwendet werden. Bei der Clonierung in Pflanzenzellsystemen können Promotoren, die von einem Pflanzenzellgenom (z. B. Hitzeschock-Promotoren, der Promotor für die kleine Untereinheit des RUBISCO; der Promotor für das Chlorophyll a/b Bindungsprotein) oder von Pflanzenviren abgeleitet sind (z, B, Wer 35S-RNA-Promotor von CaMV, der Hüllenprotein-Promotor von TMV) verwendet werden. Bei der Clonierung in Säugerzellsystemen können Promotoren, die vom Genom von Säugerzellen (z.B. Metallothionein-Promotor) oder von Säuger-Viren abgeleitet sind (z. B. der späte Adenovirus-Promotor; der Vacciniavirus 7.5K-Promotor) verwendet werden. Wenn Zelllinien erzeuet werden, die mehrere Kopien der Glucokinase codierenden Seguenz enthalten, können SV40-, BPV- und EBV- basierende Vektoren mit einem geeigneten selektierbaren Marker verwendet werden. [0020] Die Apo-, abgeleiteten und Co-Kristalle der Erfindung können mit Hilfe der in dem Fachgebiet der Proteinkri-

stallographie gut bekannten Verfahren, einschließlich Batch-, Pillussigbrücken-, Dialyse-, Dampfdiffussonsverfahren und dem Verfahren des hängenden Tropfens erhalten werden (siehe z. B. McPherson, 1982, Preparation and Analysis of Protein Crystals, John Wiley, NY, WebPherson, 1900, Eur. J. Biochem. 1899. 1–23; Webber, 1991, Adv. Protein Chent 1-1–36; Crystallization of Nucleic Acids and Proteins, herausgegeben von Arnaud Ducruix and Richard Giege, Oxford University Press; Protein Crystallization Techniques, Strategies, and Tips, herausgegeben von Terese Bergfors, International University Line, 1999). Im Allgemeinen werden die Apo- oder Co-Kristalle der Erfindung gezüchtet durch Einfonal University Line, 1999). Im Allgemeinen werden die Apo- oder Co-Kristalle der Erfindung gezüchtet durch Einfond University Line, 1999. Im Allgemeinen werden die Apo- oder Co-Kristalle der Erfindung gezüchtet durch Einfond University Line, 1999. Im Allgemeinen werden die Apo- oder Co-Kristalle der Erfindung gezüchtet durch Einfond Line versichten.

bringen eines im Wesentlichen reinen Glucckinase-Polypeptids in einen wässrigen Puffer, der ein Fällungsmittel in einer Konzentration enthäll, die gerache unterhalb derer liegt, die önüg ist um das Protein auszufällen. Dass Masser wird dann aus der Lösung durch kontrollierte Verdampfung entfernt, um Kristallisationsbedingungen zu erzeugen, die aufrechterhalten werden bis das Kristallwachstum beendet ist.

5 [0021] Bei einer bevorzugten Ausführungsform der Brindung werden Apo- oder Co-Kristalle mit Hilfe von Dampfdfülsuön gerächtent. Bei diesem Verfahren wird der Polypeptid/Pallungsmittel-Lösung ermöglicht in einem geschlesen Behälter mit einem größeren Wasserreservoir, das eine Fällungskonzentration aufweist, die für die Erzeugung des Kristalls optimal ist, zu äquibibrieren. Im Allgemeinen wird weniger als ewa 10 pla der im wessenlichen reinen Polypeptidösung mit einem gleichen Volumen der Reservoirdsung vermischt, wodurch eine Fällungsmittelkonzentration von etwa der Hälte der für die Kristallisation erfordreifschen erhalte mit Diese Lösung wird in Form eines Törjeftenen unterhalb eines Deckgläschens suspendiert, das den oberen Teil eines Reservoirs dicht verschließt. Der verschlossene Behälter wird einem Tag bei ein Alan, normalerweise etwa 2-6 Wochen, sichen gelassen bis Kristalle wachsen.

10022] Für die Kristalle der Erindung ist gefunden worden, dass hängende Tropfen, die etwa 2–5 µf Glucokinase (O-22 mg/ml n 20 nmM Tris, pdf 17.1, gemessen bei Raumiemperatur, 50 mM Nat.(.) 50 mM Glucose, 10 mM DTT und gegebenenfalls ().2 mM EDITA) und eine gleiche Menge Reservoirlösung (16–25% Gew/Nol. Polyethylenglykol mit einem mittleren Molekulargewicht von etwa 8000 bis etwa 10000 Dalton, 0,1 0,2 M Tris oder Bistris oder Hepes oder Ammoniumphosphar-Puffer, pH 6,9–75, 8–10 mM DTT, 0-39% gestäntigte Glucose) enthalten und etwa 3–4 Wochen bei 4–6°C über 0,5 bis 1,0 ml Reservoir-Puffer suspendiert wurden, Kristalle bereitstellten, die für hochauflösende Körntenstrukturanalyse geeignet werzen. Besonders bevorzuge Bedfungingen waren: etwa 2–5 µf Glucokinase (10 mg/ml in 20 mM Tris, pH 7,1, gemessen bei Raumiemperatur, 50 mM NaCl, 50 mM Glucose, 10 mM DTT und gegebenenfalls (),2 mM EDITA) und eine gleiche Menge Reservoirisbung (22,5% Gew/Nol. Polyethylenglykol mit einem mittleren Molekulargewicht von etwa 10000 Dalton, 0,1 M Tris, pH 7,08,10 mM DTT, 20% Glucose) wurden über 0,5 bis 1,0 ml Reservoir-Puffer etwa 3–4 Wochen bei 4–6°C sassendier.

[0023] Das optimale Verfahren zur Züchtung von Kristallen, die groß genug sind um damit Daten zu sammeln, ums fasste ein reisse Aufstreifen von 3-4 μl PorteiniStung auf dem Deckgläschen, gefolgt vom Aufstreifen von 3-4 μl Wannendissung auf den verlängerten Tropfen des Proteins unter Bildung eines Tröpfichens, das wie der Buchstabe "X" geformt war. Vor der Entdeckung der gekreuzen Tropfenenktik liederen die meissten Tropfen Schauer aus kleinen Kristallen, die für den Zweck der Datensammlung nicht groß genug waren. Durch die gekreuzen Tropfen wird ermöglicht, dass sich Gradienten von Protein um Fällungssmittel bliden, wenn sich die beiden Lösungen langsam vermischen und die reso sultierende Kinetik der Kristallkeinhildung und des -wachstums sind optimal zur Zuchtung einer kleinen Anzahl großer Kristalle in jedem gekreuzen Tropfen. Einfaches Zusammenmischen von Protein- umf Eillungsmittel-Lösungen in einem einzelnen runden Tropfen erzugt oft eine Überfülle von Keinnen, die zu einer endgültigen Größe wuchsen, die zum Zweck der Datensammlung zu klein sit. Die Kristalle erscheinen gewöhnlich 5 Tage nach dem Ansetzen. Die Kristalle wachsen in i om won bezagonaten Bipyramiteen, die zu pischerweise Dimensionen von 0.2-0.2-0.04 mm erreichen, ob-

35 wohl oftmals größere Kristalle beobachtet werden. Fig. 1 zeitg gezüchtete Kristalle. [0024] Die Kristalle können vor der Datensammlung eingefroren werden. Die Kristalle komen vor der Datensammlung eingefroren werden. Die Kristalle komen vor der Datensammlung eingefroren werden. Die Kristalle vor 16-20% und PEG 1000 aufgebracht bis 25% oder (d) Gitycerin zugesetzt zu 15-20%, (c) Einylenglykol zugesetzt zu 10-20% und PEG 1000 aufgebracht bis 25% oder (d) Gitycerin zugesetzt zu 15% vor Frost geschützt werden. Die Kristalle werden entweder kurz in ein Frostschutzmittel eingetwacht oder für Zeitspannen von einem Tig im Frostschutzmittel eingeweicht. Das Einfrieren erfolgt durch Eintauchen des Kristalls in einem Bad aus flüssigem Stickstoff oder durch Einbringen des Kristalls in einen Storm aus Stickstoffgas bei 100 kristalls verhanden.

[0025] Die Mosaikstreuung der gefrorenen Kristalle konnte manchmal durch Umkristallsieren ("annealing") vermindert werden, wobei der kalte Stickstoffstrom kurzzeitig blockiert wird, wodurch dem gefrorenen Kristall ermöglicht wird, für einen Moment aufzusauen bevor er im Stickstoffgasstrom erneut gefriert. Ein anderes Verfahren, das bei der Datensammlung manchmal hilfreich war, war eher eines der Enden der bewagonalen Bipyramide als den Mittelteil im Röntgenstrahl zu zentrieren. Die Mosaikstreuung kann manchmal mil Hilft diesse Verfahrens reduziert werden.

[0026] Die Beugungsdaten, die sich typischerweise bis 2,7 Å erstreckten, wurden von den gefrorenen Kristallen auf dem Synchroton Beautline X8C der National Synchroton Light Source in Brookhaven, New York, gesammelt. Unter opimalen Bedingungen wurden Daten aufgenommen, die sich bis 2,2 Å erstrecken. Siehe Fig. 3 und 4 für die Auflösung. Die Raumgruppe der Kristalle wurde als Po(5)22 während dem Lauf für die Auflösung der Kristallstruktur bestimmt. Die Kristalle haben die Elementarzell-Dimensionen a = b = 9,62+ $^{\circ}$ - $^{\circ}$

[0027] Der Fachmann wird natürlich erkennen, dass die ohen beschriebenen Kristallisationsbedingungen variiert werden können. Soliebe Variationen Können alleine oder in Kombination verwendet werden und sehißelne ein: Polypeptid55 lösungen, die Polypeptid-konzentrationen zwischen 1 mg/ml und 60 mg/ml enthalten, alle im Handel erhältlichen Puffersysteme, die den pH-Wert von etwa 6,5 bis 7,6 aufrechtentalen können. This-HCL-Konzentrationen zwischen 10 mM
und 200 mM. Dithiothreit-Konzentrationen zwischen 0 mM und 20 mM, vorzugsweise zwischen 8 und 10 mM, den
Austaussch von Dithiothreit durch p-Morcapiochtanol oder andere in der Fachwelt bekannte, äquivalente Glucosekonzentrationen zwischen 0 %E euk. Viol. und 30% Gew. Vol., oder der Austaussch von Glucose durch andere Zucker von denen
60 bekannt ist, dass sie Glucokinase binden und Reservoirlösungen die Polyethylenglykol (PEG)-Konzentrationen zwisschen etwa 10% und etwa 30% enthalten, Polyethylenglykol mittlerer Molekulagewichte zwischen etwa 1000 und etwa
20000 Dalton, alle im Handel erhältlichen Puffersysteme, die den pH-Wert von etwa 6,5 bis etwa 7,6 aufrechterhalten
können. Dithiothreit-Konzentrationen zwischen 0 mM und 20 mM, den Austausch von Olithorheit durch p-Mercaptoder anderer zucker von den bekannt ist, dass sie Glucokinase binden und die Temperatur legt im Bereirek von 4 und

[0028] Die abgeleiteten Kristalle der Erfindung können durch Einweichen der Apo- oder Co-Kristalle in der Mutterlauge, die Salze der Schwermetallatome enthält, gemäß dem Fachmann bekannter Verfahren der Röntgenkristallographie erhalten werder

[10029] Die Co-Kristalle der Brfindung können durch Binweichen eines Apo-Kristalls in Mutterlauge, die einen Liganden enthält, der an der allosterischen Stelle binder, erhalten werden oder kann durch O-Kristallisseren des Glucokinesen polyeppidis in Anwesenheit von einem oder mehreren Liganden, die an der allosterischen Stelle binden, erhalten werden. Co-Kristalle werden vorzugsweise mit einem Glucokinaseaktivator erzeugt, offenbart in: US Pat. Nr. 6,230,05t; US Pat. Amm. 09/873,2506, eingereicht am 2.1. März 2000; US Pat. Amm. 09/675,781, eingereicht am 28. September 2000; US Pat. Amm. 09/874,66, eingereicht am 2.6. April 2001; US Pat. Amm. 09/874,68, eingereicht am 2.5. April 2001; US Pat. Amm. 09/874,68,20, eingereicht am 1. Mair 2001; US Pat. Amm. 09/874,68,21, eingereicht am 1. Mair 2001; US Pat. Amm. 09/804,68,20, eingereicht am 1. Mair 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Mair 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 1. Am 2001; US Pat. Amm. 09/804,68,21, eingereicht am 2

[0030] Die hierin beschriebenen Verfahren zum Erhalt der dreidimensionalen Strukturen der kristallinen Glucokinasen, sowie der Atomstrukturkoordinaten sind in dem Erabgebiet gut bekannt (siehe, z. B., D.E. McRee, Practical Protein Crystallogrand), heraussegeben von Academie Press. San Diese (1993), und die darin züteren Referenzen).

[0031] Die Kristalle der Erindung und insbesondere die davon erhaltenen Atomstrukturkoordinaten finden eine heite Anwendung. Zum Beispiel sind die hierin beschriebenen Kristalle und Strukturkoordinaten insbesondere zur Idenlägerung von Verbindungen nützlich, die Glucokinasen aktivieren, als ein Weg im Hinblick auf die Entwicklung neuer Therapeutika. Eine solche Verbindung ist 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionanid und pharmazeutisch annehmbare Salze davon. Aus diesen Verbindungen können Arzeintmittel entwickelt werden und die Verbindungen können zur Herstellung eines Medikaments verwendet werden, das diese Verbindung zur Behandlung von Hyperglykämie bei Th-ril Diabetes umfasst.

19032] Die hierin beschriebenen Strukturkoordinaten können als Phasemmodelle zur Bestimmung der Kristallstrukturen zusätzlicher, nativer oder mutierter Glucokinasen verwendet werden, ebenso können die Strukturen der Co-Kristalle
solcher Glucokinasen mit daran gebundenen allesterischen Infibilioren oder Aktivatoren bestimmt werden. Die Strukturkoordinaten sowie Modelle der davon erhaltenen dreidimensionalen Struktur können zur Aufklärung der auf der Lösung
basierenden Strukturen von nativen oder mutierten Glucokinasen verwendet werden, ebenso wie die über NMR erhaltene. Daher stellen die Kristalle und Akomstrukturkoordinaten der Erfindung ein zweckmässiges Mittel zur Aufklärung
der Strukturen und Funktionen der Glucokinasen zur Verfügung.

[0033] Zum Zweck der Klarheit und Diskussion werden die Kristalle der Erfindung unter Bezugnahme auf spezielle
Glucokinasen durch beispielhafte Apo-Kristalle und Co-Kristalle beschrieben. Der Fachmann wird verstehen, dass die
Prinzipien, die hier beschrieben werden, generell auf Kristalle von jeder Säuger-Glucokinase anwendbar sind, einschließlich, aber nicht begrenzt, auf die Glucokinase aus Fig. 2.

[0034] So wie hierin verwendet, bezieht sich "allosterische Stelle" im allgemeinen auf jede Ligandenbindungsstelle einer Säuger-Glucokinase, die keine aktive Stelle des Enzyms ist.

[0035] So wie hierin verwendet, bezieht sich "Apo-Kristall" auf Kristalle der Säuger-Glucokinase, die ohne gebundenen allosterischen Liganden erzeugt werden.

[0036] So wie hierin verwendet, bezieht sich "allosterischer Ligand" auf jedes Molekül, das spezifisch an der allosterischen Stelle der Säuger-Glucokinase bindet. Bei einer bevorzugten Ausführungsform der Erindung einhält der Co-Kristall der Erindung einen an der allosterischen Stelle gebundenen Liganden, ausgewählt aus der Gruppe:

N-(5-Brompyridin-2-yl)-2-(3-chlor-4-methansulfonyl-phenyl)-3-cyclopentyl-propionamid, 2-(3-Chlor-4-methansulfonyl-phenyl)-3-cyclopentyl-1-(5-irfiltormethyl-pyridin-2-yl)-propionamid, (2-5)-2-(3-cyclopentyl-2-(3-4-dichlorphenyl)-propionylaminol-thiazol-4-carbons\(\text{laremethylester},\) (22)-(2-(3-4-dichlorphenyl)-propionylaminol-thiazol-5-yl)-cocssigs\(\text{suremethylester},\) (23)-(3-(3-4-dichlorphenyl)-propionyl-urido)-essigs\(\text{suremethylester},\) (23)-(3-(3-4-dichlorphenyl)-propionyl-1-dichlorphenyl)-propionyl-1-dichlorphenyl-propionyl-2-(3-4-dichlorphenyl-pyridin-4-yl-N-thiazol-2-yl-propionamid)\(\text{dichlorphenyl-propionyl}-3-(3-4-dichlorphenyl-pyridin-4-yl-N-thiazol-2-yl-propionamid)\(\text{dichlorphenyl-pyridin-4-yl-N-thiazol-2-yl-propionamid}\)

[0037] Bei einer weiteren bevorzugten Ausführungsform der Erfindung wird die Verbindung, die ein Ligand ist, der an der allosterischen Stelle der Glucokinase bindet, durch Analysieren der Strukturkoordinaten des Co-Kristalls der Erfindung identifiziert.

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[0038] Die Erfindung betrifft auch eine Verbindung

und ein pharmazeutisch verträgliches Salz davon.

[9039] Weiterhin wird mit der Efrindung ein Arzneimittel bereitgestellt, das die hierin beschriebenen Verbindungen umfasst. Diese Verbindungen betreffen Verbindungen, die durch Analysieren der Strukturdaten des Co-Kristalls wie hierin beschrieben identifiziert werden, wobei die Verbindungen Liganden sind, die an der allosterischen Stelle der Gluckinase binden. Besonders bevorzugt ist ein Arzneimittel, das die Verbindung und ein pharmazeutisch verträgliches Stalt davon unfässet.

[0040] Die hierin beschriebenen Verbindungen und Arzneimittel sollen vorzugsweise zur Behandlung von Hyperglyk-

ämie bei Tvp II Diabetes eingesetzt werden. Insbesondere werden die Verbindungen zur Verwendung als therapeutischer Wirkstoff zur Reduzierung von Hyperglykämie bei Typ II Diabetes hierein offenbart.

Beispiele

Beispiel 1

Expression und Reinigung der Glucokinase

Expression von GK

[0041] Die Glucokinase (GK) wurde als Glutathion S-Transferase (GST)-Fusionprotein in Escherichia coli exprimiert. Die Aminosäuresequenz des Fusionsproteins ist in Fig. 2 angegeben. Das Expressionskonstrukt basiert auf dem Vektor pGEX-3X von Pharmacia, wie in Y. Liang, P. Kesavan, L. Wang, K. Niswender, Y. Tanizawa, M.A. Permutt, M.A. Magnuson, F.M. Matschinsky, Biochem, J. 309, 167 (1995) beschrieben. Das Konstrukt codiert eines der beiden Leber-Isozyme der menscHichen GK. Die GST-Markierung ist am N-Terminus des Konstrukts und ist durch eine Faktor-Xa-Spaltsteile von der codierenden Sequenz von GK getrennt. Nach der Reinigung des GST-Fusionsproteins wurde die GNT-Fusionsmarkierung mit Faktor Xa-Protease entfernt, die auch fünf Reste vom N-Terminus der GK entfernt.

Reinigung der GK

[10042] E. coli Zellen, die GST-GK exprimieren wurden in Lysepuffer (50 mM Tris, 200 mM NaCl, 5 mM EDTA. 5 mM DTT, 1% NP-40, pH 7, 7) in Anwesenheit von Proteaseinhibitoren suspendiert, mit Lysozym bei 200 µ/ml 30 Minuten bei Raumtemperatur inkubiert und 4 x 30 sek, bei 4°C beschallt. Nach dem Zentrifugieren, um unlösliches Mate-25 rial zu entfernen, wurde der Überstand auf Glutathion-Sepharose geladen, mit Lysepuffer und dann mit Lysepuffer minus NP-40 gewaschen. GST-GK wurde mit Lysepuffer (minus NP-40), der 50 mM D-Glucose und 20 nnM Glutathion enthielt eluiert. Das eluierte Protein wurde konzentriert und in 20 mM iris, 100 mM NaCl, 0,2 mM EDTA, 50 mM D-Glucose, 1 mM DTT, pH 7,7 dialysjert, Faktor Xa wurde bei einem Proteinverhältnis von 1: 100 GST-GK zugesetzt, gefolgt von der Zugabe von CaCl, bis 1 mM und die Probe wurde bei 4°C 48 Stunden inkubiert. Die Probe wurde der Glutathi-30 onsepharose zugesetzt und die ungebundene Fraktion gesammelt und konzentriert. Die Probe wurde dann mit Benzamidinsepharose inkubiert, um Faktor Xa zu entfernen und die ungebundene Fraktion wurde gesammelt und auf eine Q-Sepharosesäule, die mit 25 mM Bistris-Propan, 50 mM NaCl, 5 mM DTT, 50 mM D-Glucose und 5% Glyzerin (pH 7.0) äquilibriert war geladen. Das Protein wurde mit einem NaCl-Gradienten von 50-400 mM eluiert. Fraktionen, die die gereinigte GK enthielten, wurden vereinigt, konzentriert und filtriert.

Beispiel 2

Erzeugung des Apo-Kristalls

40 [0043] 4 μl Glucokinase und 4 μl Fällungsmittel wurden vermischt und gegen die Fällungslösung bei 4°C äquilibriert. Die Glucokinaselösung bestand aus 22 mg/ml Glucokinase, hergestellt in Beispiel 1, in 20 mM Hepes pH 7,5, 50 mM NaCl, 10 mM DTT, und 50 mM Glucose. Das Fällungsmittel bestand aus 22,5% PEG 10000, 0,1 M Tris pH 7,08, 10 mM DTT, 20% Glucose; die Fällungslösung enthielt Saatkristalle für die Mikrosaat der Tröpfchen. Kristalle erschienen in den Tröpfehen nachdem die Kristallisationsplatten bei 4°C stehen gelassen wurden.

Beispiel 3

Erzeugung des Co-Kristalls mit 3-Cyclopentyl-2-Pyridin-4-yl-N-thiazol-2-yl-propionamid 3(a)

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[0044] 4 µl Glucokinase und 4 µl Fällungsmittel wurden vermischt und gegen die Fällungslösung bei 4°C äquilibriert. Die Glucokinaselösung bestand aus 13 mg7 ml Glucokinase, hergestellt in Beispiel 1, in 20 mM Tris pH 7,0, 50 mM NaCl, 10 mM DTT, 50 mM Glucose, und dem Glucokinaseaktivator 3-Cyclopentyl-2-Pyridin-4-yl-Nthiazol-2-yl-propionamid bei einer fünffachen Konzentration von derjenigen des Proteins. Das Fällungsmittel bestand aus 22,5% PEG10000, 0,1 M Tris pH 7,08, 10 mM DTT und 20% Glucose. Kristalle erschienen in den Tropfen, nachdem die Kristallisationsplatten bei 4°C stehen gelassen wurden.

3(b)

[0045] Alternativ wurden Kristalle wie in Beispiel 3(a) gezüchtet, jedoch mit den folgenden Änderungen: anstelle von 4 μl Glucokinase und 4 μl Fällungsmittel wurden jeweils 2 μl verwendet; die Glucokinaselösung enthielt 11 mg/ml Glucokinase in Tris-Puffer bei pH 7,08 anstelle von pH 7,0; die Glucokinaselösung beinhaltete 0,2 mM EDTA: anstelle von 22.5% PEG10000 als Fällungsmittel wurden 18% PEG8000 verwendet; die Fällungsmittellösung enthielt Saatkristalle 65 für die Mikrosaat der Tröpfehen.

3(c)

[0046] Bei einer anderen Alternative wurden Kristalle wie in Beispiel 3(a) gezüchtet, jedoch mit den folgenden Änderungen: anstelle von 4 µl Glucokinase und 4 µl Fällungsmittel wurden jeweils 2 µl verwendet; die Glucokinaselösung enthielt 11 mg/ml Glucokinase in Tris-Puffer bei pH 7.08 anstelle von pH 7.0; die Glucokinaselösung beinhaltete 0,2 mM EDTA; anstelle von 22,5% PEG 10000 als Fällungsmittel wurden 20% PEG8000 verwendet; die Fällungsmittel-lösune enthielt Saakristalle für die Mikrossat der Tötöfehen.

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[9047] Bei noch einer anderen Alternative wurden Kristalle wie in Beispiel 3(a) gezüchtet, jedoch mit den folgenden Anderungen; anstelle vor 4 uf Uitockinase und 4 uf Fällungsmittel wurden jeweils 2 uf verwendet; die Glucokinaselösung entlieit 12 mg/ml Glucokinase in Tris-Puffer bei pH 7.08 anstelle von pH 7.0.6 die Glucokinaselösung beinhaltete O.2 mM BDF14; anstelle von 22.55 PEG10000 orwendet; Glucose war als Bestandteil des Fällungsmittels nicht vorhanden; die Fällungsmittellösung enthielt Saakristalle für die Mikrosaat der 15 Tröofchen.

3(c)

[0048] Bei noch einer weiteren Alternative wurden Kristalle wie in Beispiel 3(a) gezüchtet, jedoch mit den folgenden 20 Änderungen: die Glucokinaselösung enthielt 11 mg/ml Glucokinase in Tris-Puffer bei pH 7,1 anstelle von 7,0; die Glucokinaselösung beinhaltete 0,2 mM EDTA; anstelle von 22,5% PEG10000 als Fällungsmittel wurden 25% PEG10000 verwendet.

3(f)

[0049] Bei noch einer weiteren Alternative wurden Kristalle, wie in Beispiel 3(a) gezüchett, jedoch mit den folgenden Änderungen: die Glucokinaseiösung enthielt 11 mg/ml Glucokinasei in Tris-Puffer bei pH 7,1 anstelle pH 7,0; die Glucokinaseiösung beinhaltete 0,2 mM EDTA: anstelle von 22,5% PEG10000 als Fällungsmittel wurden 21,25% PFG10000 verwendet; anstelle von Fällungsmittel das mit Tris auf pH 7,08 gepuffert wurde, wurde Fällungsmittel verwendet, das mit Tris auf pH 7,08 gepuffert wurde, wurde Fällungsmittel verwendet, das mit Tris auf pH 7,08 gepuffert wurde.

3(g)

[0050] Bei noch einer weiteren Alternative wurden Kristalle wie in Beispiel 3(a) gezüchtet, jedoch mit den folgenden 35 Anderungen: die Glucokinaseidsung enthielt 12 mg/ml Glucokinasei in Tris-Puffer bei pH 7,08 anstelle von 7,0; die Gilucokinaseidsung beinhaltete (2, 2 mM EDTA; anstelle von Fällungsmittel, das mit Tris auf pH 7,08 gepuffert wurde, wurde Fällungsmittel verwendet, das mit Hepes auf pH 6,89 gepuffert wurde; anstelle von 20% Glucose im Fällungsmittel wurde 200 mM Glucose verwendet.

3(h)

[0051] Bei noch einer weiteren Alternative wurden Kristalle wie in Beispiel 3(a) gezüchte, jedoch mit den folgenden Änderungen: die Glucokinaselösung enthielt 12 mg/nl Glucokinase in Tris-Puffer bei pH 7,08 anstelle von 7,0; die Glucokinaseiosung beinhaltete 0,2 mM EDTA; anstelle von Fällungsmittel, das mit 0,1 M Tris auf pH 7,08 gepuffert war, wurde Fällungsmittel verwendet, das mit 0,2 M Amoniumphosphat auf pH 7,03 gepuffert wurde; anstelle von 20% Glucose im Fällungsmittel vier 0,0 mM Glücose verwendet.

3(i)

[0052] Bei noch einer weiteren Alternative wurden Kristalle wie in Beispiel 3(a) gezüchtet, jedoch mit den folgenden Änderungen: die Glucokinaselösung enthielt 10 mg/ml Glucokinasei in This-Puffer bei pH 7,08 anstelle von pH 7,0; die Glucokinaselösung beinhaltet og. 2m ME DT34, anstelle von 25; PEG10000 als EB10lagsmittet under 26; PEG10000 verwendet; anstelle von Fällungsmittel, das mit 0,1 M Tris auf pH 7,08 gepuffert war, wurde Fällungsmittel verwendet, das mit 0,2 M Tris auf pH 7,08 gepuffert war, wurde Fällungsmittel verwendet, das mit 0,2 M Tris auf pH 7,08 gepuffert war, wurde Fällungsmittel wurde 8 mM DTT verwender; Glucose war als Bestandteil im Fällungsmittel micht vorhander.

3(i)

[0053] Bei noch einer weiteren Alternative wurden Kristalle wie in Beispiel 3(a) gezüchtet, jedoch mit den folgenden 60 Änderungen: die Glucokinaselösung enthielt 12 mg/ml Glucokinasei in Tris-Puffer bei pH 7,08 anstelle von 7.0; die Glucokinaseiosung beinhaltete O.2 mM EDTIA; anstelle von 22,5% PEG(10000 ats Fallungsmittel wurde 22% PEG(300) verwendet; Glucose war als Bestandteil des Fällungsmittels nicht vorhanden; die Fällungsmittellösung enthielt Saatkristalle für die Mikrosa der Tröpfehen.

3(k)

[0054] In noch einer weiteren Alternative wurden Kristalle wie in Beispiel 3(a) gezüchtet, jedoch mit den folgenden

Änderungen: die Glucokinaselösung enthielt 11 mg/ml Glucokinase in Tris-Puffer bei pH 7,1 anstelle von 7,0; die Glucokinaselösung beinhaltete 0,2 mM EDTA; anstelle von 20% Glucose im Fällungsmittel wurden 30% Glucose verwendet.

Beispiel 4

Erzeugung des Co-Kristalls mit N-(5-Brompyridin-2-yl)-2-(3-chlor-4-methansulfonyl-phenyl)-3-cyclopentyl-propionamid

10055] Kristalle wurden wie in Beispiel 3(a) gez\(\text{ichte, mit den folgenden \tilde{Anderungen: die Glucokinase\tilde{Sung enthielt} on mg/ml Glucokinase\tilde{Inservision} in Bris-Puffer bei pH 7,1 anstelle von 7,0; die Glucokinase\tilde{Sung beinhaltet 0,2 mM EDTA; anstelle des Glucokinase\tilde{Sung beinhaltet 0,2 mM EDTA; anstelle des Glucokinase\tilde{Sung beinhaltet 0,2 mM Glucose im Brillungs-mittel wurden 20 mM Glucose verwendet.

Beispiel 5

Erzeugung des Co-Kristalls mit 2-(3-Chlor-4-methansulfonylphenyl)-3-cyclopentyl-N-(5-trifluormethyl-pyridin-2-yl)-propionamid

[0056] Kristalle wurden wie in Beispiel 3(a) gezichtet, mit den folgenden Änderungen die Glucokinase in This-Puffer bei pf. 17. anstelle von 7.0; die Glucokinase lösung beinhaltete 0.2 mM BDTA; anstelle von 7.0; die Glucokinaselösung beinhaltete 0.2 mM BDTA; anstelle von 8.0; die Glucokinaselösung den Glucokinaselativators aus Beispiel 3(a) enthielt die Glucokinaselösung den Glucokinaselativator 2-(3-Chlor-4-methansulfonyl-phenyl)-3-cyclopsupl-N-(5-trifluormethyl-pyridin-2-yl)-propionamid; anstelle von 22,5% PEG10000 als Fällingsmittel wurde 21,25% PEG10000 verwendet.

Beispiel 6

Erzeugung des Co-Kristalls mit (2S)-2-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionylamino]-thiazol-4-carbonsäuremethylester

[0057] Kristalle wurden wie in Beispiel 3(a) gezüchtet, mit den folgenden Änderungen: die Glucokinassen Ihrs-Unferbei pf. 71, anstelle von 70, die Glucokinasselksung beinhaltete (2, 2m BEDTA; anstelle des Glucokinasselksung beinhaltete (3, 2m BEDTA; anstelle des Glucokinasselksung den Glucokina

Beispiel '

Erzeugung des Co-Kristalls mit (2S)-{2-[3-Cycfopentyl-2-(3,4-dichlorphenyl)-propionylamino]-thiazol-5-yl}oxoessigsäureethylester

[0058] Kristalle wurden wie in Beispiel 3(a) gezüchtet, mit den folgenden Änderungen: die Glucokinaseläsung enthielt 10 mg/ml Glucokinase in Tris-Puffer bei pH 7,1 anstelle von 7,0; die Glucokinaselösung beinhaltete 0,2 mM EDTA; anstelle des Glucokinaseaktivators von Beispiel 3(a) enthielt die Glucokinaselösung den Glucokinaseaktivator (2S)-[2-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionylaminoj-thiazoi-5-yl]-oxo-essigs\u00e4ureethylester; anstelle von 22,5% PBG 10000 das F\u00e4llungsmittell under \u00e41,2\u00dfree BCG 10000 das F\u00e4llungsmittell under \u00e41,2\u0

Beispiel 8

Erzeugung des Co-Kristalls mit (2S)-{3-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionyl]-ureido}-essigsäuremethylester

55 [0699] Kristalle wurden wie in Beispiel 3(a) gezüfentet, mit den folgenden Änderungen: die Glueckinaselitsung enthielt 9 mg/ml Glueckinase in Tris-Puffer bei pH 7,08 anstelle von 7,0; die Glueckinaselösung beinhaltete 0,2 mM EDTA; anstelle des Glueckinaseaktivators von Beispiel 3(a) enthielt die Glueckinaselösung den Glueckinaseaktivator (2S)-[3-[3-Cyclopentyl-2-(3-4-dichlorphenyl)-propionyl]-ureido]-essigsäuremethylester; anstelle von 20% Gluecose im Fällungsmittel wurde 200 mM Gluecose verwendet.

Beispiel 9

Erzeugung des Co-Kristalls mif (2S)-1-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionyl]-3-(3-hydroxypropyl)-harnstoff

65 [0060] Kristalle wurden wie in Beispiel 3(a) gezichtett, mit den folgenden Änderungen; die Glucokinaselösung enthielt 14 mg/m Glucokinase in Fire Fuffer bei pl 17/9.8 anstelle von 70; die Glucokinaselösung beinbaltete 0,2 mM EDITA; anstelle des Glucokinaselösunge den Glucokinaselösung den Glucokinasel

mittel wurde 200 mM Glucose verwendet.

Beispiel 10

Erzeugung des Co-Kristalls mit (2S)-{3-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionyl]-ureido}-essigsäureethylester

[0061] Kristalle wurden wie in Beispiel 3(a) gezülehtet, mit den folgenden Änderungen; die Glucokinassiäsung enthielt 4 mg/ml Glucokinase in Tris-Puffer bei pH 7,08 anstelle von 7,0; die Glucokinaselösung beinhaltete 0,2 mM EDTA; anstelle des Glucokinaselativator von Beispiel 3(a) enthielt die Glucokinaselativator (28)-(3-3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionyl-purido)-essigsäureethylester; anstelle von Fällungsmittel, das mit Tris an pH 7,08 gepuffert wurde, wurden mit Tris auf pH 7,08 gepufferts Fällungsmittel verwendet.

Beispiel 11

Synthese von 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamid

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[0062] 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamid kann unter Verwendung gutbekannter organischer Syntheseverfahren nach dem folgenden Reaktionsschema hergestellt werden:

[0063] 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-yl-propionamid ist als allosterischer Aktivator der Glucokinase und zur Unterstützung der Erzeugung von Glucokinase-Co-Kristallen nützlich.

9

SEOUENZPROTOKOLL

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Met	Leu	Gly	Gly	Cys	Pro	Lys	Glu	Arg	Ala	Glu	Ile	Ser	Met	Leu	Glu	
				85					90					95		15
Gly	Ala	Val	Leu	Asp	Ile	Arg	Tyr	Gly	Val	Ser	Arg	Ile	Ala	Tyr	Ser	
			100					105					110			20
Lys	Asp	Phe	Glu	Thr	Leu	Lys	Val	Asp	Phe	Leu	Ser	Lys	Leu	Pro	Glu	
		115					120					125				
Met	Leu	Lys	Met	Phe	Glu	Asp	Arg	Leu	Cys	His	Lys	Thr	Tyr	Leu	Asn	25
	130					135					140					
Gly	Asp	His	Val	Thr	His	Pro	Asp	Phe	Met	Leu	Tyr	Asp	Ala	Leu	Asp	30
145					150					155					160	
Val	Val	Leu	Tyr	Met	Asp	Pro	Met	Cys	Leu	Asp	Ala	Phe	Pro	Lys	Leu	35
				165					170					175		
Val	Cys	Phe	Lys	Lys	Arg	Ile	Glu	Ala	Ile	Pro	Gln	Ile	Asp	Lys	Tyr	40
			180					185					190			40
Leu	Lys	Ser	Ser	Lys	Tyr	Ile	Ala	Trp	Pro	Leu	Gln	Gly	Trp	Gln	Ala	
		195					200					205				45
Thr	Phe	Gly	Gly	Gly	Asp	His	Pro	Pro	Lys	Ser	Asp	Leu	Ile	Glu	Gly	
	210					215	- 1-			٠	220					50
Arg	Gly	Ile	His	Met	Pro	Arġ	Pro	Arg	Ser	Gln	Leu	Pro	Gln	Pro	Asn	
225					230					235					240	55
Ser	Gln	Val	Glu	Gln	Ile	Leu	Ala	Glu	Phe	Gln	Leu	Gln	Glu	Glu	Asp	
				245					250					255		
Leu	Lys	Lys	Val	Met	Arg	Arg	Met	Gln	Lys	Glu	Met	Asp	Arg	Gly	Leu	60

				260					265					270		
	Arg	Leu	Glu	Thr	His	Glu	Glu	Ala	Ser	Va1	Lys	Met	Leu	Pro	Thr	Tyr
5			275					280					285			
	Val	Arg	Ser	Thr	Pro	Glu	Gly	Ser	Glu	Val	Gly	Asp	Phe	Leu	Ser	Leu
10		290					295					300				
	Asp	Leu	Gly	Gly	Thr	Asn	Phe	Arg	Val	Met	Leu	Val	Lys	Val	Gly	Glu
15	305					310					315					320
	Gly	Glu	Glu	Gly	Gln	Trp	Ser	Val	Lys	Thr	Lys	His	Gln	Met	Tyr	Ser
20					325					330					335	
20	Ile	Pro	Glu	Asp	Ala	Met	Thr	Gly	Thr	Ala	Glu	Met	Leu	Phe	Asp	Tyr
				340					345					350		
25	Ile	Ser	Glu	Cys	Ile	Ser	Asp	Phe	Leu	Asp	Lys	His	Gln	Met	Lys	His
			355					360					365			
30	Lys	Lys	Leu	Pro	Leu	Gly	Phe	Thr	Phe	Ser	Phe	Pro	Va1	Arg	His	Glu
		370					375					380				
35	Asp	Ile	Asp	Lys	Gly	Ile	Leu	Leu	Asn	Trp	Thr	Lys	Gly	Phe	Lys	Ala
	385	1				390					395					400
	Ser	Gly	Ala	Glu	Gly	Asn	Asn	Val	Val	Gly	Leu	Leu	Arg	Asp	Ala	Ile
40					405					410					415	
	Lys	Arg	Arg	G1y	Asp	Phe	Glu	Met	Asp	Val	Val	Ala	Met	Val	Asn	Asp
45				420					425					430		
	Thr	Val	Ala	Thr	Met	Ile	Ser	Суѕ	Tyr	Tyr	Glu	Asp	His	Gln	Cys	Glu
50			435					440			-		445			
	Val	Gly	Met	Ile	Val	Gly	Thr	Gly	Cys	Asn	Ala	Cys	Tyr	Met	Glu	Glu
55		450					455					460				
33	Met	Gln	Asn	Val	Glu	Leu	Val	Glu	Gly	Asp	Glu	Gly	Arg	Met	Cys	Val
	465					470					475					480
60	Asn	Thr	Glu	Trp	Gly	Ala	Phe	Gly	Asp	Ser	Gly	Glu	Leu	Asp	Glu	Phe

				485					490					495		
Leu	Leu	Glu	Tyr	Asp	Arg	Leu	Va1	Asp	Glu	Ser	Ser	Ala	Asn	Pro	Gly	5
			500					505					510			,
Gln	Gln	Leu	Tyr	Glu	Lys	Leu	Ile	Gly	Gly	Lys	Tyr	Met	Gly	Glu	Leu	
		515					520					525				10
Val	Arg	Leu	Val	Leu	Leu	Arg	Leu	Va1	Asp	G1u	Asn	Leu	Leu	Phe	His	
	530					535					540				_	15
Gly	Glu	Ala	Ser	Glu	Gln	Leu	Arg	Thr	Arg	Gly	Ala	Phe	Glu	Thr	Arg	
545					550					555					560	20
Phe	Val	Ser	Gln	Va 1	Glu	Ser	Asp	Thr	Gly	Asp	Arg	Lys	Gln	Ile	Tyr	
				565					570					575		
Asn	Ile	Leu	Ser	Thr	Leu	Gly	Leu	Arg	Pro	Ser	Thr	Thr	Asp	Cys	Asp	25
			580					585					590			
Ile	Val	Arg	Arg	Ala	Cys	Glu	Ser	Val	Ser	Thr	Arg	Ala	Ala	His	Met	30
		595					600					605				
Сув	Ser	Ala	Gly	Leu	Ala	Gly	Va1	Ile	Asn	Arg	Met	Arg	Glu	Ser	Arg	35
	610					615					620					
	Glu	Asp	Val	Met		Ile	Thr	Val	Gly	Val	Asp	Gly	Ser	Val	Tyr	40
625					630					635					640	
Lys	Leu	His	Pro		Phe	Lys	G1u	Arg	Phe	His	Ala	Ser	Val	Arg	Arg	
_				645					650					655		45
Leu	Thr	Pro		Cys	Glu	Ile	Thr			Glu	Ser	Glu	Glu	Gly	Ser	
			660				•	665		-			670			50
GIY	Arg		Ala	Ala	Leu	Val		Ala	Val	Ala	Cys	Lys	Lys	Ala	Cys	
N - 1		675					680					685				55
Met	Leu	GIY	GIn													
	690															60
							Pa	tentans	prüche							-
a	und b	sind vo	n 79,0	2 Å bis	80,22		der Kı	ristall d	lie Eler	nentar	zell-Dii	nensio	nen au	fweist:		
C	und β	sind 9	3 Å bis 0°; und	325,0	3 A;											65
	ist 120 md P6(:		ymmet	rie hat.												

13

Co-Kristall der Säuger-Glucokinase und ein Ligand, der an der allosterischen Stelle der Glucokinase gebunden ist, wobei der Co-Kristall die Elementarzell-Dimensionen aufweist;

a und b sind von 79,02 Å bis 80,22 Å; c ist von 318,03 Å bis 325,03 Å;

α und β sind 90°; und

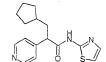
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y ist 120°; und P6(5)22-Symmetrie hat.

- Verfahren zur Co-Kristallisation von Säuger-Glucokinase und einem allosterischen Liganden der Glucokinase, wobei das Verfahren umfasst;
 - (a) Bereitstellen einer gepufferten wässrigen Lösung von 9 bis 22 mg/ml der Säuger-Glucokinase;
 - (b) Hinzufügen eines molaren Überschusses des allosterischen Liganden zur wässrigen Lösung der Säuger-Glucokinase: und
 - (c) Züchten von Kristallen mittels Dampfdiffusion unter Verwendung einer gepufferten Reservoirlösung zwischen etwa 10% und etwa 30% PEG, etwa 0% Gew./Vol. und etwa 30% Gew./Vol. Glucose und zwischen 0 und 20 mM DTT, worin das PEG ein mittleres Molekulargewicht zwischen etwa 1,000 und etwa 20,000 aufweist.
 - 4. Verfahren nach Anspruch 3, worin der Schritt (c) des Züchtens der Kristalle mittels Dampfdiffusion umfasst:
 - (a) Aufstreifen der gepufferten wässrigen Lösung der Säuger-Glucokinase mit zugesetztem allosterischem Liganden auf einer Oberfläche zur Erzeugung eines verlängerten Tröpfehens der Proteinlösung, und
 - (b) Aufstreifen von einer etwa gleichen Menge der gepufferten Reservoirlösung über das verlängerte Tröpfchen der Proteinlösung unter Bildung eines kombinierten Trönfchens, geformt wie der Buchstabe "X".
 - Co-Kristall nach Anspruch 2, wobei der Ligand ausgewählt ist aus der Gruppe:
- N-(5-Brompyridin-2-yl)-2-(3-chlor-4-methansulfonyl-phenyl)-3-cyclopentylpropionamid, 2-(3-Chlor-4-methansulfonyl-phenyl)-3-cyclopentyl-N-(5-trifluormethyl-pyridin-2-yl)-propionamid, (2S}-2-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionylamino]-thiazol-4-carbonsäuremethylester, (2S)-{2-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-25 propionylamino]-thiazol-5-yl]oxoessigsäureethylester, (2S)-{3-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionyl]ureido}-essigsäuremethylester, (2S)-1-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionyl]-3-(3-hydroxypropyl)harnstoff, (2S)-{3-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionyl]-ureido}-essigsäureethylester, 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-ylpropionamid.
- Verfahren nach Anspruch 3 oder 4, wobei der Ligand ausgewählt ist aus der Gruppe:
 - N-(5-Brompyridin-2-yl)-2-(3-chlor-4-methansulfonyl-phenyl)-3-cyclopentylpropionamid, 2-(3-Chlor-4-methansulfonyl-phenyl)-3-cyclopentyl-N-(5-trifluormethyl-pyridin-2-yl)-propionamid, (2S)-2-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionylamino]-thiazol-4-carbonsäuremethylester, (2S)-{2-[3-Cyclopentyl-2-(3,4-dichlorphenyl)propiony lamino]-thiazol-5-yl]oxoessigsäureethy lester, (2S)-{3-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionyl]-
- 35 ureido}-essigsäuremethylester. (2S)-1-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionyl]-3-(3-hydroxypropyl)harnstoff, (2S)-{3-[3-Cyclopentyl-2-(3,4-dichlorphenyl)-propionyl]-ureido}-essigsäureethylester, 3-Cyclopentyl-2-pyridin-4-yl-N-thiazol-2-ylpropionamid.
 - Kristall hergestellt mittels dem Verfahren nach Anspruch 3, 4 oder 6.
- 8. Verbindung identifiziert durch Analysieren der Strukturkoordinaten des Co-Kristalls nach Anspruch 2, wobei die Verbindung ein Ligand ist, der an der allosterischen Stelle der Glucokinase bindet. 40 9. Verbindung



und ein pharmazeutisch verträgliches Salz davon.

- Arzneimittel, umfassend die Verbindung nach Anspruch 8.
- 11. Arzneimittel nach Anspruch 10, worin die Verbindung der Verbindung nach Anspruch 8 entspricht,
- 12. Verwendung der Verbindung nach Anspruch 8 oder 9 zur Behandlung von Hyperglykämie bei Typ II Diabetes,
- 13. Verbindung nach Anspruch 8 oder 9, zur Verwendung als therapeutischer Wirkstoff, insbesondere zur Reduzierung von Hyperglykämie bei Typ II Diabetes.
- 14. Verfahren zur Herstellung eines Arzneimittels umfassend das Vermischen einer Verbindung identifiziert durch Analysieren der Strukturkoordinaten des Co-Kristalls nach Anspruch 2, wobei die Verbindung ein Ligand ist, der an die allosterische Stelle der Glucokinase bindet oder umfassend das Vermischen der Verbindung nach Anspruch 9 mit einem pharmazeutisch verträglichen Träger.

Hierzu 63 Seite(n) Zeichnungen

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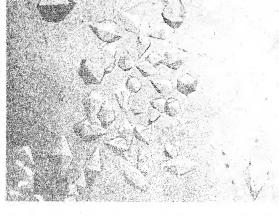
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- Leerseite -

ZEICHNUNGEN SEITE 1 Nummer: DE 102 59 786 A1

Int. Cl.7: C 12 N 9/12 Offenlegungstag. 17. Juli 2003



Figur 1

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Figur 2: Die Aminosäuresequenz des GST-GK Fusionsprotein. Die GST-Sequenz wurde dem GenBank Eintrag U13852 entnommen. Der Rest 229 des Fusionsproteins ist der erste Rest von GK.

- 1 MSPILGYWKI KGLVQPTRLL LEYLEEKYEE HLYERDEGDK WRNKKFELGL EFPNLPYYID
- 61 GDVKLTQSMA IIRYIADKHN MLGGCPKERA EISMLEGAVL DIRYGVSRIA YSKDFETLKV
- 121 DFLSKLPEML KMFEDRLCHK TYLNGDHVTH PDFMLYDALD VVLYMDPMCL DAFPKLVCFK
- 181 KRIEAIPQID KYLKSSKYIA WPLQGWQATF GGGDHPPKSD LIEGRGIHMP RPRSQLPQPN
- 241 SQVEQILAEF QLQEEDLKKV MRRMQKEMDR GLRLETHEEA SVKMLPTYVR STPEGSEVGD
- 301 FLSLDLGGTN FRVMLVKVGE GEEGQWSVKT KHQMYSIPED AMTGTAEMLF DYISECISDF
- 361 LDKHQMKHKK LPLGFTFSFP VRHEDIDKGI LLNWTKGFKA SGAEGNNVVG LLRDAIKRRG
- 421 DFEMDVVAMV NDTVATMISC YYEDHQCEVG MIVGTGCNAC YMEEMQNVEL VEGDEGRMCV
- .481 NTEWGAFGDS GELDEFLLEY DRLVDESSAN PGQQLYEKLI GGKYMGELVR LVLLRLVDEN
- 541 LLFHGEASEQ LRTRGAFETR FVSQVESDTG DRKQIYNILS TLGLRPSTTD CDIVRRACES
- 601 VSTRAAHMCS AGLAGVINRM RESRSEDVMR ITVGVDGSVY KLHPSFKERF HASVRRLTPS
- 661 CEITFIESEE GSGRGAALVS AVACKKACML GO



Figur 3

Figur 4

		2.1	om	A.A.					
Atom	No	T		Тур	A.A.#	х	Y	z	OCC B .
MOTA	-1121		СВ	SER	8	-0.421	63.744	24.899	1.00 50.68
ATOM	- 2		OG	SER	8	-0.752	63.605	23.524	1.00 50.85
MOTA		3	C	SER	8	1.865	64.216	24.094	1.00 50.72
ATOM		4	0	SER	8	2.308	63.644	23.102	1.00 51.79
ATOM		5	N	SER	8	1.473	63.793	26.507	1.00 50.36
ATOM		6	CA	SER	8	1.057	63.446	25.120	1.00 50.55
MOTA		7	N	GLN	9	2.041	65.515	24.314	1.00 49.84
MOTA		8	CA	GLN	9	2.831	66.312	23.385	1.00 48.95
ATOM		9	CB	GLN	9	2.983	67.745	23.895	1.00 49.08
MOTA	1	0	CG	GLN	9	3.676	68.686	22.925	1.00 50.25
ATOM	1:		CD	GLN	9	3.206	70.127	23.085	1.00 51.06
MOTA	1:		OE1	GLN	9	2.037	70.433	22.846	1.00 51.38
MOTA	1	3	NE2	GLN	9	4.112	71.017	23.499	1.00 51.44
ATOM	1.	4	C	GLN	9	4.190	65.633	23.294	1.00 48.56
ATOM	1		0	GLN	. 9	4.884	65.741	22.285	1.00 48.75
ATOM	1		N	VAL	.10	4.560	64.926	24.361	1.00 47.77
MOTA	1		CA	VAL	10	5.823	64.198	24.392	1.00 46.87
MOTA	1		CB	VAL	10	6.293	63.902	25.842	1.00 46.39
MOTA	1		CG1	VAL	10	7.303	62.782	25.841	1.00 46.41
MOTA	2		CG2	VAL	10	6.952	65.135	26.436	1.00 46.79
MOTA	2		C	VAL	10	5.616	62.885	23.653	1.00 46.17
ATOM	2		0	VAL	10	6.521	62.384	22.991	1.00 46.18
ATOM	2		N	GLU	11	4.423	62.317	23.768	1.00 45.28
ATOM	2		CA	GLU	11	4.159	61.071	23.069	1.00 45.19
MOTA	2		CB	GLU	11	2.905	60.393	23.616	1.00 45.21
ATOM	2		CG	GLU	11	3.105	59.709	24.967	1.00 46.05
ATOM	2		CD	GLU	11	4.224	58.664	24.957	1.00 46.30
ATOM	2			GLU	11	4.350	57.918	23.948	1.00 46.28
ATOM	2		OE2	GLU	11	4.963	58.583	25.972	1.00 45.66
ATOM	3		С	GLU	11	4.002	61.345	21.580	1.00 44.48
ATOM ATOM	3		O N	GLU	11 12	4.068	60.430	20.755 21.239	1.00 44.48
ATOM	3		CA	GLN	12	3.646	62.614 62.996	19.845	1.00 42.86
ATOM	3		CB	GLN	12	2.972	64.368	19.715	1.00 44.49
MOTA	3		CG	GLN	12	2.833	64.840	18.259	1.00 46.49
ATOM	3		CD	GLN	12	1.986	66.099	18.113	1.00 47.74
MOTA	3			GLN	12	2.055	66.799	17.088	1.00 48.30
MOTA	3		NE2	GLN	12	1.174	66.388	19.131	1.00 47.51
MOTA	3		c	GLN	12	5.014	63.023	19.192	1.00 41.14
ATOM	4		ŏ	GLN	12	5.139	62.739	18.002	1.00 41.76
MOTA	4		N	ILE	13	6.038	63.360	19.971	1.00 38.51
ATOM		2	CA	ILE	13	7.398	63.388	19.450	1.00 36.48
ATOM	4		СВ	ILE	13 -	8.274	64.351	20,261	1.00 35.85
ÁTOM	4	4	CG2		13	9.731	64.228	19.827	1.00 35.71
ATOM	4	5	CG1		13	7.740	65,777	20.079	1.00 35.77
ATOM	4	6	CD1	ILE	13	8.584	66.867	20.710	1.00 35.91
ATOM	4	7	С	ILE	13	8.018	61.981	19.452	1.00 36.01
ATOM	4	8	0	ILE	13	8.572	61.528	18.442	1.00 35.99
ATOM	4	9	N	LEU	14	7.903	61.288	20.580	1.00 34.88
ATOM	5	0	CA	LEU	14	8.430	59.934	20.711	1.00 33.91
MOTA	5	1	CB	LEU	14	8.230	59.432	22.141	1.00 33.29
ATOM	5	2	CG	LEU	14	8.853	60.321	23.215	1.00 33.43
MOTA	5	3	CD1	LEU	14	8.510	59.781	24.594	1.00 33.04
MOTA	5	4	CD2	LEU	14	10.354	60.398	23.001	1.00 33.04

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	gui 4							
» move	55		T DIT	14	7.766	58.957	19.730	1.00 33.55
ATOM		C	LEU					
ATOM	56	0	LEU	14	8.208	57.812	19.578	1.00 33.21
ATOM	57	N	ALA	15	6.710	59.403	19.065	1.00 32.69
MOTA	58	CA	ALA	15	6.021	58.551	18.104	1.00 32.59
ATOM	59	CB	ALA	15	4.628	59.104	17.821	1.00 31.95
MOTA	60	C	ALA	15	6.838	58.449	16.808	1.00 32.79
ATOM	61	0	ALA	15	6.664	57.519	16.018	1.00 33.05
MOTA	62	N	GLU	16	7.746	59.395	16.599	1.00 32.33
MOTA	63	CA	GLU	16	8.575	59.369	15.403	1.00 32.74
MOTA	64	CB	GLU	16	9.566	60.531	15.401	1.00 34.23
MOTA	65	CG	GLU	16	8.950	61.910	15.298	1.00 38.39
ATOM	66	CD	GLU	16	10.017	62.998	15.162	1.00 41.11
ATOM	67	OE1	GLU	16	10.445	63.269	14.012	1.00 40.68
ATOM	68	OE2	GLU	16	10.438	63.562	16.212	1.00 42.77
ATOM	69	C	GLU	16	9.369	58.073	15.279	1.00 31.93
ATOM	70	0	GLU	16	9.570	57.568	14.179	1.00 33.41
ATOM	71	N	PHE	17	9.841	57.539	16.401	1.00 30.37
ATOM	72	CA	PHE	17	10.640	56.321	16.369	1.00 27.71
MOTA	73	CB	PHE	17	11.346	56.129	17.711	1.00 26.32
ATOM	74	CG	PHE	17	12.309	57.230	18.045	1.00 24.22
MOTA	75	CD1		17	11.846	58.500	18.389	1.00 23.88
ATOM	76	CD2	PHE	17	13.680	57.010	17.981	1.00 22.24
ATOM	77	CE1		17	12.741	59.531	18.660	1.00 22.63
MOTA	78	CE2	PHE	17	14.574	58.027	18.250	1.00 21.23
MOTA	79	CZ	PHE	17	14.105	59.291	18.589	1.00 22.01
MOTA	80	c	PHE	17	9.836	55.077	16.012	1.00 27.77
ATOM	81	ō	PHE	17	10.400	54.004	15.802	1.00 27.38
MOTA	82	N	GLN	18	8.517	55.213	15.957	1.00 28.12
ATOM	83	CA	GLN	18	7.684	54.080	15.593	1.00 29.17
ATOM	84	CB	GLN	18	6.216	54.484	15.599	1.00 30.98
ATOM	85	CG	GLN	18	5.446	54.017	16.806	1.00 32.94
ATOM	86	CD	GLN	18	4.152	54.785	16.974	1.00 34.65
ATOM	87	OE1		18	3.389	54.976	16.014	1.00 37.17
ATOM	88	NE2		18	3.892	55.228	18.190	1.00 33.67
ATOM	89	C	GLN	18	8.068	53.602	14.193	1.00 28.97
ATOM	90	õ	GLN	18	8.471	54.399	13.346	1.00 28.83
ATOM	91	N	LEU	19	7.931	52.298	13.971	1.00 29.02
MOTA	92	CA	LEU	19	8.235	51.659	12.704	1.00 29.94
ATOM	93	CB	LEU	19	9.641	51.069	12.749	1.00 29.78
ATOM	94	CG	LEU	19	10.782	51.813	12.037	1.00 30.77
ATOM	95		LEU	19	10.886	53.251	12.477	1.00 30.67
ATOM	96		LEU	19	12.083	51.087	12.339	1.00 32.05
ATOM	97	C	LEU	19	7.199	50.549	12.511	1.00 31.41
ATOM	98	ō	LEU	19	7.288	49.484		1.00 31.35
ATOM	99	N	GLN	20	6.205	50.801	11.663	1.00 32.64
ATOM	100	CA	GLN	20	5.153	49.817	11.422	1.00 34.95
ATOM	101	CB	GLN	20	4.024	50.413	10.570	1.00 35.78
ATOM	102	CG	GLN	20	3.301	51.622	11.175	1.00 37.65
ATOM	103	CD	GLN	20	3.048	51.486	12.669	1.00 39.03
ATOM	104		GLN	20	2.603	50.441	13.152	1.00 40.92
ATOM	105	NE2		20	3.324	52.552	13.410	1.00 40.04
ATOM	106	C	GLN	20	5.692	48.568	10.730	1.00 35.83
ATOM	107	o	GLN	20	6.827	48.547	10.247	1.00 36.56
ATOM	108	N	GLU	21	4.864	47.531	10.681	1.00 36.52
ATOM	109	CA	GLU	21	5.240	46.279	10.062	1.00 37.80
ATOM	110	CB	GLU	21	4.024	45.357	9.998	1.00 37.80
ATOM	111	CG	GLU	21	4.298	43.898	9.625	1.00 42.88
ATOM	112	CD	GLU	21	4.568	43.009	10.844	1.00 44.63
ATOM	113		GLU	21	4.540	41.758	10.699	1.00 45.40
ATOR	113	OET	GHO	21	4.540	41./38	20.033	1.00 43.40

Figur 4

MOTA	114	OE2	GLU	21	4.810	43.564	11.943	1.00 45.89
ATOM	115	C	GLU	21	5.770	46.549	8.654	1.00 38.20
MOTA	116	0	GLU	21	6.892	46.183	8.324	1.00 38.71
ATOM	117	N	GLU	22	4.972	47.208	7.826	1.00 38.54
ATOM	118	CA	GLU	22	5.386	47.478	6.457	1.00 39.08
ATOM	119	CB	GLU	22	4.308	48.267	5.703	1.00 40.61
ATOM	120	CG	GLU	22	3.123	47.406	5.313	1.00 43.51
ATOM	121	CD	GLU	22	3.556	46.039	4.773	1.00 45.80
ATOM	122		GLU	22	4.243	45.999	3.719	1.00 46.20
ATOM	123	OE2	GLU	22	3.215	45.007	5.414	1.00 46.87
ATOM	124	С	GLU	22	6.711	48.197	6.359	1.00 38.74
ATOM	125	0	GLU	22	7.482	47.954	5.423	1.00 39.26
MOTA	126	N	ASP	23	6.988	49.084	7.308	1.00 37.74
ATOM	127	CA	ASP	23	8.258	49.795	7.276	1.00 37.23
MOTA	128	CB	ASP	23	8.356	50.779	8.437	1.00 38.62
ATOM	129	CG	ASP	23	7.240	51.789	8.427	1.00 40.46
ATOM	130		ASP	23	7.104	52.508	7.408	1.00 41.26
ATOM	131		ASP	23	6.495	51.861	9.438	1.00 41.77
ATOM	132	C	ASP	23	9.371	48.760	7.382	1.00 35.54
MOTA	133	Ö	ASP	23	10.267	48.698	6.536	1.00 35.43
MOTA	134	N	LEU	24	9.294	47.937	8.420	1.00 33.31
ATOM	135	CA	LEU	24	10.288	46.910	8.631	1.00 32.04
ATOM	136	CB	LEU	24	9.898	46.062	9.842	1.00 31.35
ATOM	137	CG	LEU	24	9.920	46.801	11.196	1.00 31.20
MOTA	138		LEU	24	9710	45.815	12.343	1.00 29.48
ATOM	139		LEU	24	11.253	47.526	11.367	1.00 31.51
MOTA	140	C	LEU	24	10.509	46.041	7.385	1.00 31.61
ATOM	141	0	LEU	24	11.645	45.723	7.049	1.00 31.67
ATOM	142	N	LYS	25	9.434	45.673	6.693	1.00 31.58
ATOM	143	· CA	LYS	25	9.551	44.863	5.486	1.00 31.41
ATOM	144	CB	LYS	25	8.186	44.347	5.061	1.00 31.41
MOTA	145	CG	LYS	25	7.574	43.372	6.033	1.00 34.39
ATOM	146	CD	LYS	25	6.224	42.901	5.531	1.00 36.61
ATOM	147	CE	LYS	25	5.414	42.232	6.640	1.00 38.71
ATOM	148	NZ	LYS	25	3.978	42.232	6.235	1.00 39.39
ATOM	149	C	LYS	25	10.166	45.679	4.352	1.00 31.50
ATOM	150	ō	LYS	25	10.969	45.170	3.568	1.00 30.92
ATOM	151	N	LYS	26	9.784	46.947	4.261	1.00 31.82
ATOM	152	CA	LYS	26	10.332	47.819	3.229	1.00 32.63
ATOM	153	CB	LYS	26	9.695	49.203	3.315	1.00 33.38
ATOM	154	CG	LYS	26	10.053	50.129	2.177	1.00 35.11
ATOM	155	CD	LYS	26	9.424	51.502	2.400	1.00 37.48
ATOM	156	CE	LYS	26	9.364	52.312	1.104	1.00 37.40
ATOM	157	NZ	LYS	26	8.706	53.645	1.307	1.00 42.62
ATOM	158	c	LYS	26	11.845	47.919	3.441	1.00 32.91
MOTA	159	ŏ	LYS	26	12.614	48-012	2.479	1.00 32.90
ATOM	160	N	VAL	27	12.265	47.901	4.705	1.00 33.16
ATOM	161	CA	VAL	27	13.687	47.956	5.046	1.00 33.43
ATOM	162	CB	VAL	27	13.903	48.281	6.555	1.00 32.58
ATOM	163		VAL	27	15.335	47.960	6.963	1.00 32.13
ATOM	164	CG2		27	13.622	49.755	6.818	1.00 31.04
ATOM	165	C	VAL	27	14.305	46.586	4.727	1.00 33.90
ATOM	166	Ö	VAL	27	15.323	46.482	4.036	1.00 33.83
ATOM	167	N	MSE	28	13.668	45.536	5.223	1.00 34.26
ATOM	168	CA	MSE	28	14.140	44.193	4.983	1.00 34.84
ATOM	169	CB	MSE	28	13.072	43.198	5.393	1.00 35.83
ATOM	170	CG	MSE	28	13.456	41.784	5.144	1.00 38.88
ATOM	171	SE	MSE	28	12.108	40.670	5.608	1.00 45.40
ATOM	172	CE	MSE	28	11.054	40.713	4.095	1.00 42.96
01.	112	015	MOS	20	11.034	-0.713	4.033	2.00 42.50

Figur 4

ATOM	173	С	MSE	28	14.465	44.016	3.505	1.00 35.32
ATOM	174	0	MSE	28	15.571	43.621	3.144	1.00 35.22
MOTA	175	N	ARG	29	13.495	44.331	2.655	1.00 36.22
MOTA	176	CA	ARG	29	13.665	44.191	1.218	1.00 36.59
ATOM	177	CB	ARG	29	12.352	44.520	0.509	1.00 37.37
ATOM	178	CG	ARG	29	11.223	43.542	0.827	1.00 38.96
MOTA	179	CD	ARG	29	9.913	43.960	0.152	1.00 40.89
ATOM	180	NE	ARG	29	8.760	43.281	0.744	1.00 42.88
ATOM	181	CZ	ARG	29	7.621	43.889	1.081	1.00 43.80
ATOM	182	NH1		29	7.475	45.201	0.881	1.00 43.07
ATOM	183		ARG	29	6.631	43.188	1.636	1.00 44.12
ATOM	184	С	ARG	29	14.814	45.008	0.625	1.00 36.30
ATOM	185	0	ARG	29	15.615	44.469	-0.133	1.00 35.58
MOTA	186	N	ARG	30	14.906	46.296	0.948	1.00 36.85
ATOM	187	CA CB	ARG	30 30	15.008	47.091	0.410	1.00 38.41
ATOM ATOM	188 189	CG	ARG	30	15.944 14.676	48.543	0.894	1.00 39.31 1.00 41.96
ATOM	190	CD	ARG	30	14.076	50.763	0.933	1.00 44.07
ATOM	191	NE	ARG	30	13.415	51.384	0.995	1.00 45.48
ATOM	192	CZ	ARG	30	13.179	52.628	1.416	1.00 45.93
ATOM	193	NH1	ARG	30	14.175	53.403	1.810	1.00 45.92
ATOM	194		ARG	30	11.937	53.091	1.467	1.00 45.68
ATOM	195	C	ARG	30	17.338	46.461	0.843	1.00 39.05
MOTA	196	ō	ARG	30	18.286	46.404	0.061	1.00 38.99
MOTA	197	N	MSE	31	17.408	45.999	2.092	1.00 39.11
MOTA	198	CA	MSE	31	18.615	45.348	2.596	1.00 38.96
MOTA	199	CB	MSE	31	18.374	44.784	4.002	1.00 40.43
MOTA	200	CG	MSE	31	19.512	43.922	4.599	1.00 42.62
MOTA	201	SE	MSE	31	21.083	44.819	5.027	1.00 48.46
ATOM	202	CE	MSE	31	20.438	45.988	6.389	1.00 45.46
ATOM	203	C	MSE	31	18.901	44.209	1,633	1.00 38.25
ATOM	201	0	MSE	31	19.973	44.132	1.038	1.00 38.18
ATOM	205	N	GLN	32	17.915	43.334	1.478	1.00 37.93
ATOM	206	CA	GLN	32	18.037	42.199	0.589	1.00 37.33
MOTA	207	CB	GLN GLN	32 32	16.708 16.219	41.475	0.480	1.00 36.41 1.00 37.04
ATOM	209	CD	GLN	32	15.304	39.723	1.561	1.00 37.04
ATOM	210		GLN	32	15.740	38.682	1.072	1.00 38.23
ATOM	211		GLN	32	14.027	39.874	1.912	1.00 37.39
ATOM	212	c	GLN	32	18.475	42.641	-0.791	1.00 37.81
MOTA	213	ō	GLN	32	19.215	41.929	-1.466	1.00 37.79
MOTA	214	N	LYS	33	18.019	43.819	-1.205	1.00 38.80
ATOM	215	CA	LYS	33	18.362	44.345	-2.516	1.00 39.85
ATOM	216	CB	LYS	33	17.525	45.588	-2.830	1.00 40.63
ATOM	217	CG	LYS	33	17.591	45.992	-4.298	1.00 42.21
ATOM	218	CD	LYS	33	16.924	47 _336	-4.561	1.00 43.78
ATOM	219	CE	LYS	33	17.160	47.803	-6.006	1.00 44.42
ATOM	220	NZ	LYS	33	16.639	49.187	-6.256	1.00 44.23
ATOM	221	C	LYS	33	19.843	44.695	-2.574	1.00 40.37 1.00 40.53
ATOM	222	N	LYS	33 34	20.519	44.411	-3.564	1.00 40.53
ATOM ATOM	223	CA	GLU	34	20.331	45.312 45.712	-1.500 -1.378	1.00 40.39
ATOM	225	CB	GLU	34	21.730	45.712	-0.179	1.00 41.24
ATOM	225	CG	GLU	34	21.229	46.841	-0.179	1.00 41.24
ATOM	227	CD	GLU	34	21.476	48.506	-1.741	1.00 42.21
ATOM	228	OE1		34	22.650	48.810	-2.063	1.00 42.30
ATOM	229	OE2		34	20.493	48.613	-2.507	1.00 43.29
ATOM	230	C	GLU	34	22.667	44.528	-1.221	1.00 40.87
ATOM	231	ō	GLU	34	23.770	44.527	-1.767	1.00 41.06

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Figur 4

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ATOM	23	32	N	MSE	35	22.233	43.534	-0.456	1.00 41.15
MOTA	2:		CA	MSE	35	23.038	42.350	-0.232	1.00 41.36
ATOM		34	CB	MSE	35				
						22.289	41.354	0.648	1.00 41.62
ATOM	2:		CG	MSE	35	22.320	41.711	2.117	1.00 43.28
MOTA		36	SE	MSE	35	21.428	40.506	3.120	1.00 46.51
ATOM	23	37	CE	MSE	35	22.217	38.947	2.587	1.00 45.63
MOTA	2:	38	C	MSE	35	23.376	41.701	-1.554	1.00 41.91
ATOM	2:	39	0	MSE	35	24.532	41.367	-1.824	1.00 42.73
MOTA	24	40	N	ASP	36	22.367	41.533	-2.395	1.00 42.15
ATOM		41.	CA	ASP	36	22.593	40.898	-3.675	1.00 41.96
ATOM		12	CB	ASP	36	21.264	40.633	-4.369	1.00 43.56
		43			36				
MOTA			CG	ASP		21.446	39.947	-5.699	1.00 45.91
MOTA		44	OD1		36	21.821	40.652	-6.675	1.00 46.71
MOTA		45		ASP	36	21.232	38.707	-5.754	1.00 46.76
MOTA		46	C	ASP	36	23.502	41.717	-4.578	1.00 41.03
MOTA	2	47	0	ASP	36	24.406	41.178	-5.217	1.00 40.61
ATOM	2	48	N	ARG	37	23.257	43.021	-4.620	1.00 40.36
ATOM	2	49	CA	ARG	37	24.034	43.937	-5.446	1.00 39.76
ATOM	2	50	CB	ARG	37	23.498	45.355	-5.283	1.00 39.56
ATOM		51	CG	ARG	37	22.252	45.621	-6.112	1.00 40.04
ATOM		52	CD	ARG	37	21.465			1.00 41.19
ATOM		53		ARG	37		46.815	-5.590	
			NE			22.278	48.002	-5.307	1.00 41.70
ATOM		54	CZ	ARG	37	22.938	48.711	-6.221	1.00 42.38
ATOM		55		ARG	37	22.899	48.362	-7.505	1.00 42.59
MOTA		56		ARG	37	23.615	49.792	-5.851	1.00 41.94
ATOM		57	С	ARG	37	25.524	43.908	-5.152	1.00 39.94
ATOM	2	58	0	ARG	37	26.335	43.732	-6.059	1.00 40.39
MOTA	2	59	N	GLY	38	25.893	44.076	-3.890	1.00 39.94
ATOM	2	60	CA	GLY	38	27.305	44.063	-3.557	1.00 39.60
ATOM		61	С.	GLY	38	27.933	42.689	-3.699	1.00 39.23
MOTA		62	ŏ	GLY	38	29.163	42.546	-3.695	1.00 39.59
MOTA		63	N	LEU	39	27.087	41.677	-3.834	1.00 38.16
ATOM		64	CA	LEU	39	27.545			
MOTA		65	CB		39		40.307	-3.960	1.00 37.65
				LEU		26.428	39.376	-3.495	1.00 35.76
ATOM		66	CG	LEU	39	26.821	38.029	-2.900	1.00 34.52
MOTA		67	CD1		39	27.899	38.248	-1.857	1.00 33.52
ATOM		68		LEU	39	25.606	37.348	-2.284	1.00 32.44
ATOM		69	С	LEU	39	27.931	39.989	-5.407	1.00 39.20
ATOM	2	70	0	LEU	39	28.594	38.980	-5.681	1.00 39.88
ATOM	2	71	N	ARG	40	27.537	40.866	-6.329	1.00 40.51
ATOM	2	72	CA	ARG	40	27.809	40.656	-7.751	1.00 41.77
ATOM	2	73	CB	ARG	40	26.494	40.686	-8.526	1.00 42.80
ATOM		74	CG	ARG	40	25.735	39.392	-8.377	1.00 44.75
MOTA		75	CD	ARG	40	24.257	39.551	-8.636	1.00 46.47
ATOM		76	NE	ARG	40	23.639	38.239	-8.797	1.00 48.71
ATOM		77	CZ	ARG	40	22.331	38-034	-8.890	1.00 40.71
ATOM		78			40				
			NH1	ARG		21.497	39.064	~8.831	1.00 51.43
ATOM		79	NH2	ARG	40	21.861	36.804	-9.060	1.00 50.45
MOTA		80	C	ARG	40	28.802	41.623	-8.374	1.00 42.16
MOTA		81	0	ARG	40	28.783	42.819	-8.097	1.00 42.42
ATOM		82	N	LEU	41	29.650	41.087	-9.247	1.00 42.03
MOTA	2	83	CA	LEU	41	30.689	41.864	-9.902	1.00 42.00
ATOM	2	84	CB	LEU	41	31.307	41.044	-11.041	1.00 42.00
ATOM	2	85	CG	LEU	41	32.577	41.650	-11.660	1.00 41.78
ATOM		86		LEU	41	33.638	41.836	-10.583	1.00 40.20
ATOM		87	CD2		41	33.087	40.747	-12.773	1.00 41.95
ATOM		88	C	LEU	41	30.278	43.237	-12.773	1.00 42.57
ATOM		89	Ö	LEU	41	30.278		-10.428	1.00 42.57
ATOM		90					44.243		
ATOM	2	30	N	GLU	42	29.219	43.292	-11.227	1.00 43.03

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Figur 4

	Ü						
ATOM	291	CA GLU	42	28.788	44.562	-11.803	1.00 44.63
ATOM	292	CB GLU	42	27.494	44.369	-12,607	1.00 43.97
ATOM	293	CG GLU	42	26.436	43.533	-11,922	1.00 44.02
ATOM	294	CD GLU	42	26.546	42.057	-12.248	1.00 43.71
ATOM	295	OE1 GLU	42	27.673	41.527	-12.245	1.00 45.13
ATOM	296	OE2 GLU	42	25.504	41.416	-12.496	1.00 43.50
ATOM	297	C GLU	42	28.616	45.714	-10.805	1.00 46.21
ATOM	298	O GLU	42	28.963	46.860	-11.103	1.00 46.22
ATOM	299	N THR	43	28.105	45.413	-9.616	1.00 47.90
ATOM	300	CA THR	43	27.873	46.443	-8.608	1.00 49.10
ATOM	301	CB THR	43	26.370	46.533	-8.285	1.00 48.63
ATOM	302	OG1 THR	43	25.772	45.242	-8.465	1.00 47.66
ATOM	303	CG2 THR	43	25.679	47.531	-9.192	1.00 48.90
ATOM	304	C THR	43	28.629	46.226	-7.302	1.00 50.94
ATOM	3 0 5	O THR	4.3	28.481	47.008	-6.362	1.00 51.52
MOTA	306	N HIS	44	29.456	45.185	-7.249	1.00 52.58
ATOM	307	CA HIS	44	30.204	44.854	-6.037	1.00 53.89
ATOM	308	CB HIS	44	31.210	43.727	-6.311	1.00 54.68
ATOM	309	CG HIS	44	32.552	44.208	-6.775	1.00 55.77
ATOM	310	CD2 HIS	44	33.748	44.257	-6.139	1.00 55.82
ATOM	311	ND1 HIS	44	32.758	44.772	-8.017	1.00 56.36
ATOM	312	CE1 HIS	44	34.020	45.146	-8.125	1.00 56.30
ATOM	313	NE2 HIS	44	34.643	44.845	-6.999	1.00 56.06
ATOM	314	C HIS	44	30.950	46.013	-5.398	1.00 54.87
ATOM	315	O HIS	44	30.823	46.254	-4.199	1.00 55.06
ATOM	316	N GLU	45	31.724	46.732	-6.203	1.00 56.25
ATOM	317	CA GLU	45	32.540	47.826	-5.703	1.00 57.17
ATOM	318	CB GLU	45	33.618	48.180	-6.721	1.00 59.35
ATOM	319	CG GLU	45	33.146	49.127	-7.800	1.00 61.61
ATOM	320	CD GLU	45	34.107	50.279	-7.985	1.00 63.07
ATOM	321	OE1 GLU	45	35.228	50.038	-8.487	1.00 63.72
ATOM	322	OE2 GLU	45	33.747	51.420	-7.613	1.00 64.00
ATOM	323	C GLU	45	31.762	49.074	-5.356	1.00 56.66
ATOM	324	O GLU	45	32.295	49.985	-4.732	1.00 56.54
MOTA	325	N GLU	46	30.508	49.135	-5.772	1.00 56.24
ATOM	326	CA GLU	46	29.708	50.306	-5.456	1.00 56.37
ATOM	327	CB GLU	46	29.542	51.157	-6.704	1.00 57.92
MOTA	328	CG GLU	46	30.881	51.645	-7.212	1.00 60.77
ATCM	329	CD GLU	46	30.782	52.400	-8.515	1.00 62.28
ATCM	330	OE1 GLU	46	30.566	51.762	-9.571	1.00 62.25
ATOM	331	OE2 GLU	46	30.914	53.641	-8.474	1.00 63.95
MOTA	332	C GLU	46	28.366	49.891	-4.873	1.00 55.40
MOTA	333	O GLU	46	27.309	50.123	-5.457	1.00 55.75
ATOM	334	N ALA	47	28.440	49.264	-3.704	1.00 53.89
ATOM	335	CA ALA	47	27.273	48.783	-2.987	1.00 51.80
ATOM	336	CB ALA	47	27.140	47_280	-3.159	1.00 52.36
ATOM	337	C ALA	47	27.470	49.111	-1.524	1.00 49.98
MOTA	338	O ALA	47	28.448	48.664	-0.923	1.00 50.36
ATOM	339	N SER	48	26.553	49.894	-0.960	1.00 47.18
ATOM	340	CA SER	48	26.630	50.267	0.444	1.00 44.70
ATOM	341	CB SER	48	25.299	50.860	0.897	1.00 46.13
ATOM	342	OG SER	48	24.243	49.927	0.720	1.00 47.87
ATOM	343	C SER	48	26.965	49.041	1.287	1.00 42.45
ATOM	344	O SER	48	27.841	49.082	2.147	1.00 42.01
ATOM	345	N VAL	49	26.261	47.946	1.037	1.00 40.48
ATOM	346	CA VAL	49	26.516	46.713	1.762	1.00 38.96
ATOM	347	CB VAL	49	25.231	45.849	1.875	1.00 38.62
MOTA	348	CG1 VAL	49	25.496	44.625	2.740	1.00 38.40
ATOM	349	CG2 VAL	49	24.102	46.672	2.472	1.00 37.16

Figur 4

6								
ATOM	350	C	VAL	49	27.572	45.997	0.929	1.00 37.97
ATOM	351	0	VAL	49	27,266	45.474	-0.137	1.00 38.42
ATOM	352	N	LYS	50	28.810	45.982	1.422	1.00 36.51
ATOM	353	CA	LYS	50	29.937	45.385	0.703	1.00 34.95
ATOM	354	CB	LYS	50	31.250	45.843	1.334	1.00 35.51
ATOM	355	CG	LYS	50	31.574	47.322	1.091	1.00 36.68
MOTA	356	CD	LYS	50	30.676	48.249	1.913	1.00 39.05
MOTA	357	CE	LYS	50	30.865	48.018	3.419	1.00 39.54
MOTA	358	NZ	LYS	50	32.316	48.157	3.792	1.00 40.04
ATOM	359	C	LYS	50	30.012	43.879	0.482	1.00 33.72
ATOM	360	0	LYS	50	30.845	43.421	-0.293	1.00 33.30
ATOM	361	N	MSE	51	29.171	43.100	1.147	1.00 33.02
ATOM	362	CA	MSE	51	29.209	41.647	0.967	1.00 32.08
ATOM	363	CB	MSE	51	28.291	41.257	-0.190	1.00 34.01
ATOM	364	CG	MSE	51	26.867	41.744	-0.025	1.00 36.03
MOTA	365	SE	MSE	51	26.148	41.146	1.529	1.00 40.73
MOTA	366	CE	MSE	51	25.558	39.411	1.085	1.00 37.98
MOTA	367	C	MSE	51	30.637	41.180	0.666	1.00 30.17
ATOM	368	0	MSE	51	30.928	40.723	-0.437	1.00 30.22
ATOM	369	N	LEU	52	31.518	41.295	1.650	1.00 28.96
ATOM	370	CA	LEU	52	32.920	40.928	1.487	1.00 27.43
MOTA	371	CB	LEU	52	33.769	41.839	2.357	1.00 28.05
ATOM	372	CG	LEU	52	33.649	43.319	1.991	1.00 28.52
MOTA	373	CD1	LEU	52	34.222	44.171	3.116	1.00 28.77
MOTA	374	CD2	LEU	52	34.369	43.583	0.658	1.00 28.75
ATOM	375	C	LEU	52	33.273	39.482	1.803	1.00 26.61
ATOM	376	0	LEU	52	32.997	38.995	2.893	1.00 25.26
MOTA	377	N	PRO	53	33.911	38.774	0.844	1.00 27.04
ATOM	378	CD	PRO	53	34.270	39.142	-0.540	1.00 25.69
ATOM	379	CA	PRO-	53	34.264	37.375	1.133	1.00 27.99
MOTA	380	CB	PRO		34.807	36.864	-0.204	1.00 26.92
MOTA	381	CG	PRO	53	34.184	37.825	-1.241	1.00 25.77
MOTA	382	C	PRO	53	35.314	37.361	2.239	1.00 28.40
MOTA	383	0	PRO	53	36.152	38.271	2.317	1.00 28.36
MOTA	384	N	THR	54	35.255	36.329	3.080	1.00 29.46
ATOM	385	CA	THR	54	36.149	36.142	4.226	1.00 30.53
ATOM	386	CB	THR	54	35.317	35.951	5.502	1.00 29.48
ATOM	387	OG1		54	34.589	34.711	5.418	1.00 27.97
ATOM	388		TER	54	34.324	37.084	5.659	1.00 29.42
ATCM	389	C	THR	54	37.018	34.884	4.071	1.00 31.60
ATOM	390	0	THR	54	37.657	34.423	5.025	1.00 32.25
MOTA	391	N	TYR	5.5	37.017	34.311	2.877	1.00 32.63
ATOM	392	CA	TYR	55 55	37.763	33.089	2.615	1.00 34.41
ATOM ATOM	393 394	CB	TYR	55	39.249 39.458	33.421	2.405	1.00 32.58
	395			55			1.101	1.00 32.44
ATOM	395	CD1			39.518	35.571 36.263	1.067	1.00 32.44
ATOM	397	CE1		55 55	39.572		-0.157	1.00 32.48
ATOM	398	CD2		-55	39.467 39.516	33.492 34.172	-0.117 -1.335	1.00 31.83
ATOM ATOM	399	CZ	TYR	55	39.516	35.548	-1.351	1.00 32.18
ATOM	400	OH	TYR	55	39.566	36.200	-2.568	1.00 32.10
ATOM	400	C	TYR	55	37.559	36.200	3.637	1.00 36.06
ATOM	401	0	TYR	55	38.314	30.991	3.665	1.00 37.61
ATOM	403	N	VAL	56	36.518	30.991	4.459	1.00 37.01
ATOM	404	CA	VAL	56	36.199	31.006	5.429	1.00 39.87
ATOM	404	CB	VAL	56	35.483	31.586	6.663	1.00 38.75
ATOM	406		VAL	56	35.202	30.492	7.669	1.00 38.10
ATOM	407	CG		56	36.336	32.660	7.285	1.00 38.76
ATOM	408	C	VAL	56	35.249	30.032	4.706	1.00 42.20
111011	400	C	V ALL	50	33.649	50.032	9.700	2.00 30.20

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Figur 4

ATOM	rig	ur 4							
ATOM 410 N ARG 57 35.718 28.821 4.414 1.00 44.49 ATOM 411 CA ARG 57 35.718 28.821 4.414 1.00 44.49 ATOM 412 CB ARG 57 36.898 27.860 3.676 1.00 47.07 ATOM 412 CB ARG 57 36.898 27.880 2.499 1.00 48.02 ATOM 413 CG ARG 57 36.299 28.310 1.508 1.00 49.08 ATOM 414 CD ARG 57 36.558 27.626 0.185 1.00 49.69 ATOM 415 NB ARG 57 37.239 28.528 -0.737 1.00 49.50 ATOM 416 CZ ARG 57 37.239 28.528 -0.737 1.00 49.50 ATOM 416 CZ ARG 57 38.936 28.997 0.745 1.00 48.83 ATOM 418 NH2 ARG 57 38.915 29.978 -1.345 1.00 47.51 ATOM 420 0 ARG 57 34.810 26.695 4.449 1.00 48.57 ATOM 420 0 ARG 57 34.810 26.695 4.449 1.00 48.57 ATOM 420 0 ARG 57 34.810 26.695 4.449 1.00 48.57 ATOM 420 0 ARG 57 34.810 26.695 4.449 1.00 51.15 ATOM 421 N SER 58 33.256 26.117 3.891 1.00 51.15 ATOM 422 CA SER 58 33.2589 24.973 4.501 1.00 54.78 ATOM 420 0 ARG 57 34.810 26.310 5.500 1.00 48.65 ATOM 422 CA SER 58 31.258 24.973 4.501 1.00 54.78 ATOM 420 0 ARG 57 34.810 24.793 3.882 1.00 54.26 ATOM 420 CG SER 58 31.258 24.993 4.793 4.501 1.00 54.78 ATOM 420 CG SER 58 31.258 24.993 4.275 1.00 57.39 ATOM 425 C SER 58 33.497 22.7645 4.293 1.00 57.47 ATOM 420 CG SER 58 33.497 22.7645 4.293 1.00 57.47 ATOM 428 CG SER 58 33.697 22.645 4.293 1.00 57.47 ATOM 428 CG SER 58 33.697 22.645 4.293 1.00 57.47 ATOM 428 CG SER 58 33.697 22.645 4.293 1.00 60.71 ATOM 428 CG THR 59 35.896 22.823 1.758 1.00 60.71 ATOM 420 CG THR 59 35.896 22.823 1.758 1.00 63.73 ATOM 430 CG1 THR 59 35.592 22.740 3.16 1.00 66.71 ATOM 421 N GROW 49 CG SER 58 33.997 2.7645 4.029 1.570 1.00 63.73 ATOM 430 CG1 THR 59 36.537 22.880 4.756 1.00 67.44 ATOM 431 CG THR 59 36.537 22.880 4.756 1.00 67.74 ATOM 432 C THR 59 36.537 22.880 4.756 1.00 67.70 ATOM 431 CG THR 59 36.637 22.740 3.156 1.00 67.74 ATOM 432 C THR 59 36.637 22.740 3.156 1.00 67.74 ATOM 433 C THR 59 36.637 22.740 3.156 1.00 67.74 ATOM 430 CG1 THR 59 36.637 22.740 3.156 1.00 67.75 ATOM 430 CG1 THR 59 36.637 22.740 3.156 1.00 67.74 ATOM 430 CG1 THR 59 36.637 22.740 3.156 1.00 67.75 ATOM 430 CG THR 59 36.637 22.740 3.156 1.00 67.75 ATOM 430 CG THR 59 36.637	ATOM	409	0	JAV.	56	34 098	30 376	4 410	1 00 42 02
ATOM 411 CA ARG 57 34.896 27.860 3.676 1.00 47.07 ATOM 412 CB ARG 57 35.688 27.288 2.489 1.00 48.02 ATOM 413 CG ARG 57 36.585 27.628 2.489 1.00 48.02 ATOM 414 CD ARG 57 36.585 27.626 0.185 1.00 49.08 ATOM 415 NE ARG 57 36.555 27.626 0.185 1.00 49.08 ATOM 415 NE ARG 57 36.555 27.626 0.185 1.00 49.08 ATOM 415 NE ARG 57 38.367 29.167 -0.447 1.00 48.83 ATOM 417 NR1 ARG 57 38.936 28.997 0.745 1.00 48.13 ATOM 419 C ARG 57 38.936 29.978 -1.345 1.00 47.51 ATOM 419 C ARG 57 38.936 29.978 -1.345 1.00 47.51 ATOM 419 C ARG 57 38.915 29.978 -1.345 1.00 47.51 ATOM 419 C ARG 57 34.311 26.695 4.499 1.00 48.57 ATOM 421 N SER 58 33.256 26.117 3.891 1.00 51.15 ATOM 422 CA SER 58 32.589 24.973 4.501 1.00 54.78 ATOM 422 CA SER 58 31.254 24.993 3.891 1.00 54.26 ATOM 422 CA SER 58 31.254 24.993 3.892 1.00 54.26 ATOM 424 CG SER 58 31.254 24.993 3.892 1.00 57.39 ATOM 425 C SER 58 31.258 24.990 2.475 1.00 54.39 ATOM 425 C SER 58 33.419 23.708 4.295 1.00 57.39 ATOM 426 O SER 58 33.492 22.740 3.510 1.00 64.02 ATOM 428 CA THR 59 35.392 22.740 3.510 1.00 64.02 ATOM 428 CA THR 59 35.392 22.740 3.510 1.00 64.02 ATOM 428 CA THR 59 35.392 22.740 3.510 1.00 64.02 ATOM 428 CA THR 59 35.896 22.823 1.758 1.00 64.02 ATOM 421 CG THR 59 36.637 24.029 1.750 1.00 63.22 ATOM 423 CD THR 59 36.637 24.029 1.750 1.00 63.22 ATOM 423 CD THR 59 36.637 24.029 1.750 1.00 63.27 ATOM 423 CD THR 59 36.637 24.029 1.750 1.00 63.27 ATOM 423 CD THR 59 37.554 23.562 3.884 1.00 67.10 64.02 ATOM 431 CG THR 59 37.554 23.562 3.884 1.00 67.10 64.02 ATOM 431 CG THR 59 37.554 23.562 3.884 1.00 67.10 64.02 ATOM 432 CD THR 59 37.554 23.562 3.884 1.00 67.10 63.87 ATOM 435 CD PRO 60 35.366 21.412 5.854 1.00 70.63 ATOM 436 CA PRO 60 37.556 23.00 63.37 1.00 71.72 ATOM 437 CB PRO 60 35.366 21.412 5.854 1.00 70.63 ATOM 430 CD PRO 60 38.709 21.370 6.056 1.00 71.72 ATOM 431 CG PRO 60 37.556 23.00 63.37 1.00 71.72 ATOM 445 CD GLU 61 40.806 17.516 5.261 1.00 70.63 ATOM 445 CD GLU 61 40.806 17.516 5.261 1.00 70.63 ATOM 445 CD GLU 61 40.806 17.516 5.261 1.00 70.63 ATOM 445 CD GLU 61 40.806 1									
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Figur 4

ATOM									
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ATOM 485 OD 2 ASP 67 48.386 25.791 24.956 1.00 49.62 ATOM 486 C ASP 67 47.832 27.634 20.612 1.00 47.26 ATOM 487 O ASP 67 48.786 27.635 19.827 1.00 47.26 ATOM 488 N PHE 68 46.935 28.632 20.678 1.00 45.40 ATOM 489 CA PHE 68 46.935 28.632 20.678 1.00 45.40 ATOM 490 CA PHE 68 46.032 28.361 17.946 1.00 39.29 ATOM 491 CO PHE 68 46.032 28.361 17.946 1.00 33.76 ATOM 492 CD1 PHE 68 46.032 28.361 17.946 1.00 33.76 ATOM 493 CD2 PHE 68 45.621 27.199 18.592 1.00 33.76 ATOM 494 CE1 PHE 68 45.621 27.199 18.592 1.00 33.76 ATOM 495 CE2 PHE 68 46.468 28.772 16.623 1.00 33.76 ATOM 496 CZ PHE 68 46.469 28.772 16.623 1.00 33.76 ATOM 497 C PHE 68 46.498 27.050 15.959 1.00 37.76 ATOM 498 O PHE 68 46.998 31.096 20.514 1.00 43.33 ATOM 498 O PHE 68 46.938 31.096 20.514 1.00 43.33 ATOM 498 O PHE 68 46.395 31.147 21.621 1.00 43.27 ATOM 499 N LEU 69 47.386 32.166 19.899 1.00 43.51 ATOM 500 CA LEU 69 47.274 33.475 20.497 1.00 44.73 ATOM 501 CB LEU 69 49.166 33.4349 21.848 1.00 45.26 ATOM 502 CG LEU 69 49.166 33.4349 21.848 1.00 45.26 ATOM 503 CD1 LEU 69 49.861 33.928 22.932 1.00 46.03 ATOM 504 CD2 LEU 69 49.861 34.399 21.00 46.33 ATOM 505 C C LEU 69 48.781 34.949 21.848 1.00 45.26 ATOM 508 CA SER 70 44.274 33.899 1.00 44.79 ATOM 509 C SER 70 42.294 34.984 20.074 1.00 44.72 ATOM 501 CB LEU 69 49.813 34.394 21.848 1.00 45.26 ATOM 501 CB SER 70 44.250 36.978 20.199 1.00 44.79 ATOM 501 CB SER 70 44.250 36.978 20.199 1.00 44.79 ATOM 501 CB SER 70 44.250 36.978 20.199 1.00 44.72 ATOM 510 CB SER 70 44.250 36.978 20.199 1.00 44.73 ATOM 510 CB SER 70 44.250 36.978 20.199 1.00 44.73 ATOM 510 CB SER 70 44.250 36.978 20.199 1.00 44.73 ATOM 510 CB SER 70 44.250 36.978 20.199 1.00 44.73 ATOM 510 CB SER 70 44.250 36.978 20.199 1.00 44.73 ATOM 510 CB SER 70 44.250 36.978 20.199 1.00 44.73 ATOM 510 CB SER 70 44.250 36.978 20.199 1.00 49.90 ATOM 511 C SER 70 44.250 36.978 20.199 1.00 49.90 ATOM 512 C SER 70 44.250 36.978 20.199 1.00 49.90 ATOM 513 N LEU 71 47.088 38.997 18.499 1.00 49.90 ATOM 513 N ASP 72 43.899 40.0877 19.039 1.00 49.93 ATOM 520 C LEU 71 47	MOTA					48.381	25.452	23.751	1.00 49.34
ATOM 486 C ASP 67 47.832 27.634 20.612 1.00 47.26 ATOM 487 0 ASP 67 48.786 27.635 19.827 1.00 47.26 ATOM 488 N PHE 68 46.955 28.632 20.678 1.00 45.41 ATOM 489 C B PHE 68 46.955 28.632 20.678 1.00 45.41 ATOM 490 CB PHE 68 46.031 29.7682 19.785 1.00 45.51 ATOM 491 CC PHE 68 46.031 29.7682 19.785 1.00 43.53 ATOM 492 CD1 PHE 68 46.031 29.7682 18.667 1.00 41.17 ATOM 491 CC PHE 68 46.032 28.361 17.946 1.00 39.29 ATOM 493 CD2 PHE 68 46.632 28.361 17.946 1.00 39.29 ATOM 493 CD2 PHE 68 46.662 28.272 16.623 1.00 38.75 ATOM 493 CD2 PHE 68 46.468 28.272 16.623 1.00 38.74 ATOM 495 CE2 PHE 68 46.498 27.050 15.959 1.00 37.76 ATOM 495 CE2 PHE 68 46.986 25.983 16.619 1.00 37.76 ATOM 497 C PHE 68 46.986 25.893 16.619 1.00 37.76 ATOM 498 C PHE 68 46.986 25.893 16.619 1.00 37.76 ATOM 498 D PHE 68 46.986 25.893 16.619 1.00 43.33 ATOM 498 N LEU 69 47.386 32.156 19.889 1.00 43.33 ATOM 499 N LEU 69 47.386 32.156 19.889 1.00 43.31 ATOM 501 CB LEU 69 48.623 34.197 20.518 1.00 45.27 ATOM 501 CB LEU 69 48.623 34.197 20.518 1.00 45.26 ATOM 502 CD LEU 69 48.781 34.949 21.848 1.00 45.33 ATOM 503 CD1 LEU 69 49.811 36.072 21.748 1.00 45.36 ATOM 503 CD1 LEU 69 49.811 36.072 21.748 1.00 45.37 ATOM 505 C LEU 69 49.811 36.072 21.748 1.00 45.37 ATOM 505 C LEU 69 49.811 36.072 21.748 1.00 45.37 ATOM 507 N SER 70 42.294 34.475 20.397 1.00 44.75 ATOM 507 N SER 70 42.294 34.475 20.391 1.00 44.57 ATOM 507 N SER 70 42.294 34.481 18.470 1.00 44.58 ATOM 507 N SER 70 42.294 34.481 18.470 1.00 44.58 ATOM 509 CB SER 70 42.794 31.475 20.197 1.00 44.77 ATOM 510 CB SER 70 42.294 34.481 18.470 1.00 44.57 ATOM 511 C SER 70 44.451 37.289 21.277 1.00 44.77 ATOM 512 C SER 70 44.250 36.978 20.109 1.00 44.99 ATOM 512 C SER 70 44.250 36.978 20.109 1.00 44.97 ATOM 512 C SER 70 44.250 36.978 20.109 1.00 44.97 ATOM 513 C SER 70 44.250 36.978 20.109 1.00 49.97 ATOM 513 C C LEU 71 44.092 37.898 19.307 1.00 44.97 ATOM 514 CA LEU 71 44.092 37.898 19.307 1.00 44.97 ATOM 515 C C LEU 71 47.008 38.997 19.039 1.00 49.97 ATOM 515 C C LEU 71 47.008 38.997 18.499 1.00 49.97 ATOM 515 C	MOTA	484	OD1	ASP	67	48.201	24.287	23.365	1.00 49.37
ATOM 487 O ASP 67 48.786 27.635 19.827 1.00 47.44 ATOM 488 N PHE 68 46.955 28.632 20.678 1.00 45.41 ATOM 490 CB PHE 68 46.955 28.632 20.678 1.00 45.41 ATOM 491 CG PHE 68 46.031 29.682 18.667 1.00 41.17 ATOM 492 CD PHE 68 46.032 28.361 17.946 1.00 39.29 ATOM 493 CD2 PHE 68 46.032 28.361 17.946 1.00 39.29 ATOM 493 CD2 PHE 68 45.621 27.199 18.592 1.00 33.57 ATOM 494 CEI PHE 68 45.647 25.966 17.934 1.00 33.24 ATOM 495 CE2 PHE 68 46.468 27.050 15.995 1.00 37.31 ATOM 497 C PHE 68 46.498 27.050 15.995 1.00 37.31 ATOM 498 O PHE 68 46.988 37.050 15.995 1.00 37.31 ATOM 498 O PHE 68 46.988 31.096 20.514 1.00 43.33 ATOM 498 O PHE 68 46.938 31.147 21.621 1.00 43.33 ATOM 499 N LEU 69 47.366 32.166 19.899 1.00 43.57 ATOM 500 CA LEU 69 48.625 31.167 19.899 1.00 43.51 ATOM 501 CB LEU 69 48.625 31.167 19.889 1.00 43.51 ATOM 502 CG LEU 69 48.625 31.497 20.518 1.00 45.26 ATOM 503 CD1 LEU 69 48.625 31.97 20.518 1.00 45.26 ATOM 504 CD2 LEU 69 46.275 34.297 1.00 44.73 ATOM 505 C LEU 69 46.275 34.297 21.00 46.09 ATOM 507 C D LEU 69 46.275 34.298 19.681 1.00 45.37 ATOM 508 C LEU 69 46.275 34.288 19.681 1.00 45.37 ATOM 509 C S ER 70 42.794 33.989 20.351 1.00 45.52 ATOM 501 C LEU 69 46.275 34.281 19.681 1.00 45.37 ATOM 508 C S ER 70 42.794 33.989 19.697 1.00 44.79 ATOM 508 C S ER 70 42.697 33.899 19.697 1.00 44.79 ATOM 508 C S ER 70 42.697 33.899 19.697 1.00 44.79 ATOM 510 C SER 70 42.697 33.899 19.697 1.00 44.79 ATOM 510 C SER 70 42.697 33.899 19.697 1.00 44.79 ATOM 510 C SER 70 42.697 33.899 19.697 1.00 44.79 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.92 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.92 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 49.95 ATOM 510 C LEU 71 44.092 37.889 19.481 1.00 49.57 ATOM 510 C LEU 71 44.092 37.889 19.481 1.00 49.95 ATOM 510 C LEU 71 47.098 38.979 18.499 1.00 48.07 ATOM 510 C LEU 71 47.098 38.979 18.499 1.00 48.07 ATOM 510 C LEU 71 47.098 38.979 19.039 1.00 49.95 ATOM 520 C LEU 71 47.098 38.979 19.039 1.00 49.95 ATOM 521 C A SEP 72 40.043 40.807 20.262 1.00 49.95							25.791		1.00 49.62
ATOM 488 N PHE 68 46.955 28.632 20.678 1.00 45.41 ATOM 490 CA PHE 68 47.075 29.778 19.785 1.00 45.41 ATOM 490 CA PHE 68 46.031 29.682 19.785 1.00 43.60 ATOM 491 CG PHE 68 46.031 29.682 19.785 1.00 33.55 ATOM 492 CD1 PHE 68 46.032 28.851 17.946 1.00 33.29 ATOM 493 CD2 PHE 68 46.082 28.7719 18.592 1.00 33.55 ATOM 493 CD2 PHE 68 46.682 28.77.199 18.592 1.00 33.55 ATOM 494 CE1 PHE 68 46.682 28.79.199 18.592 1.00 33.76 ATOM 495 CE2 PHE 68 46.986 25.993 16.619 1.00 37.76 ATOM 496 CZ PHE 68 46.986 25.993 16.619 1.00 37.76 ATOM 497 C PHE 68 46.986 25.993 16.619 1.00 37.76 ATOM 498 O PHE 68 46.986 25.993 16.619 1.00 43.27 ATOM 499 N LEU 69 47.386 32.156 19.889 1.00 43.27 ATOM 500 CA LEU 69 47.386 32.156 19.889 1.00 43.27 ATOM 501 CA LEU 69 47.274 33.475 20.497 1.00 44.73 ATOM 502 CG LEU 69 48.625 34.197 20.518 1.00 45.26 ATOM 503 CD1 LEU 69 49.166 33.928 22.932 1.00 46.03 ATOM 504 CD2 LEU 69 49.166 33.928 22.932 1.00 46.03 ATOM 505 C LEU 69 49.816 30.072 27.748 1.00 45.88 ATOM 505 C LEU 69 46.275 34.278 19.681 1.00 45.62 ATOM 507 N SER 70 45.248 4.451 18.470 1.00 45.62 ATOM 509 CB SER 70 42.697 43.899 20.511 10.00 45.62 ATOM 501 C SER 70 42.697 33.899 19.44 1.00 44.73 ATOM 501 C SER 70 44.250 36.978 20.151 10.00 45.62 ATOM 501 C SER 70 44.250 36.978 20.151 10.00 45.72 ATOM 510 C SER 70 42.697 33.899 19.44 1.00 44.61 ATOM 510 C SER 70 42.697 33.899 19.44 1.00 44.61 ATOM 510 C SER 70 42.697 33.899 19.44 1.00 44.67 ATOM 510 C SER 70 42.697 33.899 19.44 1.00 44.67 ATOM 510 C SER 70 42.697 33.899 19.44 1.00 44.67 ATOM 510 C SER 70 42.697 33.899 19.44 1.00 44.67 ATOM 510 C SER 70 42.697 43.994 20.074 1.00 44.69 ATOM 510 C SER 70 42.697 33.899 19.40 10.00 44.99 ATOM 510 C SER 70 42.697 33.899 19.40 10.00 44.99 ATOM 512 C SER 70 44.250 36.978 19.100 10.00 44.99 ATOM 513 C LEU 71 44.092 39.394 19.305 1.00 49.69 ATOM 513 C LEU 71 44.092 37.893 19.100 49.09 ATOM 513 C LEU 71 44.092 37.893 19.100 49.09 ATOM 513 C C LEU 71 47.348 40.977 19.00 49.77 ATOM 513 C C LEU 71 47.348 40.977 19.00 49.79 ATOM 520 C LEU 71 47.348 40.977 19.00 4			C	ASP	67	47.832	27.634	20.612	1.00 47.26
ATOM 489 CA PHE 68 47.075 29.778 19.785 1.00 43.60 ATOM 491 CG PHE 68 46.031 29.682 18.667 1.00 41.17 ATOM 492 CD PHE 68 46.032 28.361 17.946 1.00 39.29 ATOM 493 CD PHE 68 46.032 28.361 17.946 1.00 39.29 ATOM 493 CD PHE 68 46.686 28.272 16.623 1.00 38.76 ATOM 494 CPL PHE 68 45.647 25.966 17.934 1.00 38.24 ATOM 495 CPL PHE 68 45.647 25.966 17.934 1.00 38.24 ATOM 496 CPL PHE 68 46.489 27.050 15.995 1.00 37.31 ATOM 497 C PHE 68 46.498 27.050 15.995 1.00 37.36 ATOM 497 C PHE 68 46.998 37.050 15.995 1.00 37.76 ATOM 499 N LEU 69 47.274 33.1096 20.514 1.00 43.33 ATOM 499 N LEU 69 47.386 32.166 19.899 1.00 43.51 ATOM 500 CA LEU 69 48.625 31.167 19.899 1.00 48.52 ATOM 501 CB LEU 69 48.625 34.197 20.518 1.00 45.26 ATOM 502 CG LEU 69 48.625 34.197 20.518 1.00 45.26 ATOM 503 CD LEU 69 48.625 34.197 20.518 1.00 45.26 ATOM 504 CD2 LEU 69 48.625 34.197 20.2912 1.00 46.09 ATOM 505 C LEU 69 49.166 33.298 22.292 1.00 46.09 ATOM 505 C LEU 69 49.166 33.298 22.292 1.00 46.09 ATOM 507 N SER 70 45.288 34.758 20.351 1.00 45.37 ATOM 508 CA SER 70 44.250 36.978 20.351 1.00 45.52 ATOM 509 CB SER 70 42.697 33.899 19.844 1.00 45.52 ATOM 510 CS SER 70 42.697 33.899 19.844 1.00 46.53 ATOM 510 CS SER 70 42.697 33.899 19.844 1.00 46.53 ATOM 510 CS SER 70 42.697 33.899 19.844 1.00 46.52 ATOM 510 CS SER 70 42.697 33.899 19.844 1.00 46.57 ATOM 510 CS SER 70 42.697 33.899 19.844 1.00 46.57 ATOM 510 CS SER 70 42.697 33.899 19.844 1.00 46.57 ATOM 510 CS SER 70 42.697 33.899 19.844 1.00 46.57 ATOM 510 CS SER 70 42.697 33.899 19.844 1.00 46.57 ATOM 510 CS SER 70 42.697 33.899 19.844 1.00 46.57 ATOM 510 CS SER 70 44.250 36.978 20.109 1.00 44.59 ATOM 510 CS SER 70 44.650 36.978 20.109 1.00 44.59 ATOM 510 CS SER 70 44.650 36.978 20.109 1.00 44.59 ATOM 510 CS SER 70 44.250 36.978 20.109 1.00 44.59 ATOM 510 CS SER 70 44.250 36.978 20.109 1.00 44.59 ATOM 510 CS SER 70 44.250 36.978 20.109 1.00 49.90 ATOM 510 CS SER 70 44.250 36.978 20.109 1.00 49.90 ATOM 510 CS SER 70 44.250 36.978 20.109 1.00 49.90 ATOM 510 CS SER 70 44.250 36.978 20.109 1.00 49.90 ATOM 51	MOTA	487	0	ASP	67	48.786	27.635	19.827	1.00 47.44
ATOM 489 CA PHE 68 47.075 29.778 19.785 1.00 43.50 ATOM 490 CB PHE 68 46.031 29.682 18.667 1.00 41.17 ATOM 491 CG PHE 68 46.031 29.682 18.667 1.00 41.17 ATOM 492 CD1 PHE 68 45.621 27.199 18.592 1.00 38.55 ATOM 493 CD2 PHE 68 45.621 27.199 18.592 1.00 38.75 ATOM 493 CD2 PHE 68 45.621 27.199 18.592 1.00 38.75 ATOM 495 CE2 PHE 68 46.468 28.272 16.623 1.00 38.76 ATOM 495 CE2 PHE 68 46.498 27.050 15.955 1.00 37.31 ATOM 497 C PHE 68 46.498 27.050 15.955 1.00 37.31 ATOM 498 O PHE 68 46.398 31.096 20.514 1.00 43.33 ATOM 498 O PHE 68 46.918 31.096 20.514 1.00 43.37 ATOM 499 N LEU 69 47.374 33.475 20.497 1.00 44.33 ATOM 500 CA LEU 69 47.274 33.475 20.497 1.00 44.73 ATOM 501 CB LEU 69 48.625 34.197 20.518 1.00 45.26 ATOM 502 CG LEU 69 48.781 34.994 21.848 1.00 46.33 ATOM 503 CD1 LEU 69 49.166 33.282 22.392 1.00 46.09 ATOM 505 C LEU 69 49.811 36.072 22.748 1.00 45.48 ATOM 505 C LEU 69 49.811 36.072 22.748 1.00 45.48 ATOM 505 C LEU 69 49.811 36.072 22.748 1.00 45.48 ATOM 507 N SER 70 45.282 34.758 20.351 1.00 45.75 ATOM 508 CA SER 70 45.282 34.758 20.351 1.00 45.75 ATOM 510 CS SER 70 42.594 33.899 19.844 1.00 44.25 ATOM 510 CS SER 70 44.250 36.978 20.109 1.00 44.79 ATOM 510 CS SER 70 44.250 36.978 20.109 1.00 44.92 ATOM 510 CS SER 70 44.250 36.978 20.109 1.00 44.92 ATOM 510 CS SER 70 44.250 36.978 20.109 1.00 44.92 ATOM 510 CS SER 70 44.551 37.899 12.777 1.00 44.97 ATOM 510 CS SER 70 44.551 37.899 12.777 1.00 44.57 ATOM 510 CS SER 70 44.551 37.899 12.777 1.00 44.57 ATOM 510 CS SER 70 44.552 36.978 20.109 1.00 44.92 ATOM 510 CS SER 70 44.551 37.899 12.777 1.00 44.67 ATOM 510 CS CR TO 44.951 37.899 12.777 1.00 44.67 ATOM 510 CS CR TO 44.951 37.899 12.777 1.00 44.67 ATOM 510 CS CR TO 44.951 37.899 12.777 1.00 44.67 ATOM 510 CS CR TO 44.951 37.899 12.777 1.00 44.67 ATOM 510 CS CR TO 44.951 37.899 12.777 1.00 44.67 ATOM 510 CS CR TO 44.951 38.997 18.499 1.00 49.95 ATOM 510 CS CR TO 44.951 39.942 18.7756 1.00 49.794 ATOM 510 CS CR TO 44.952 37.899 12.777 1.00 44.67 ATOM 510 CS CR TO 44.952 37.899 12.777 1.00 44.994 ATOM 510 CS CR	MOTA	488	N	PHE	68	46.955	28.632	20.678	1.00 45.41
ATOM 490 CB PHE 68 46.031 29.682 18.667 1.00 41.17 ATOM 491 CG PHE 68 46.032 28.361 17.946 1.00 39.29 ATOM 492 CD1 PHE 68 45.621 27.199 18.592 1.00 38.55 ATOM 493 CD2 PHE 68 45.621 27.199 18.592 1.00 38.55 ATOM 494 CB1 PHE 68 45.6468 28.272 16.623 1.00 38.76 ATOM 495 CB2 PHE 68 45.6467 25.966 17.934 1.00 38.24 ATOM 495 CB2 PHE 68 45.647 25.966 17.934 1.00 38.24 ATOM 495 CB2 PHE 68 45.982 7.050 15.959 1.00 37.76 ATOM 497 CP PHE 68 46.998 27.050 15.959 1.00 37.76 ATOM 497 CP PHE 68 46.998 31.147 21.621 1.00 43.27 ATOM 498 O PHE 68 46.918 31.096 20.514 1.00 43.27 ATOM 499 N LEU 69 47.386 32.167 19.889 1.00 43.31 ATOM 499 N LEU 69 47.386 32.167 19.889 1.00 43.27 ATOM 500 CA LEU 69 47.274 33.475 20.497 1.00 44.73 ATOM 501 CB LEU 69 48.625 34.197 20.518 1.00 45.27 ATOM 502 CG LEU 69 48.625 34.197 20.518 1.00 45.33 ATOM 504 CD2 LEU 69 49.166 33.928 22.932 1.00 46.03 ATOM 504 CD2 LEU 69 49.166 33.928 22.932 1.00 46.03 ATOM 505 C LEU 69 46.275 34.278 19.681 1.00 45.63 ATOM 505 C LEU 69 46.275 34.278 19.681 1.00 45.55 ATOM 507 N SER 70 45.248 4.451 18.470 1.00 45.75 ATOM 509 CB SER 70 44.177 35.528 19.681 1.00 45.75 ATOM 509 CB SER 70 44.250 36.978 20.109 1.00 44.73 ATOM 509 CB SER 70 44.250 36.978 20.109 1.00 44.99 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.72 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.99 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.99 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.99 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.72 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.92 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.93 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.93 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.93 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.93 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.93 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.93 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.93 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.93 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.93 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.93 ATOM 510 C SER 70 44	MOTA	489	CA	PHE	68	47.075	29.778		
ATOM 491 CC PHE 68 46.032 28.361 17.946 1.00 39.29 ATOM 492 CD1 PHE 68 45.621 27.199 18.592 1.00 38.55 ATOM 493 CD2 PHE 68 45.621 27.199 18.592 1.00 38.55 ATOM 493 CD2 PHE 68 45.624 27.199 18.592 1.00 38.55 ATOM 494 CEI PHE 68 45.647 25.966 17.934 1.00 38.24 ATOM 495 CE2 PHE 68 46.498 27.050 15.955 1.00 37.31 ATOM 495 CE2 PHE 68 46.498 27.050 15.955 1.00 37.31 ATOM 497 C PHE 68 46.988 31.096 20.514 1.00 43.33 ATOM 498 O PHE 68 46.988 31.096 20.514 1.00 43.33 ATOM 498 O PHE 68 46.988 31.096 20.514 1.00 43.37 ATOM 499 N LEU 69 47.374 33.1475 20.497 1.00 44.73 ATOM 500 CA LEU 69 47.274 33.475 20.497 1.00 44.73 ATOM 501 CB LEU 69 48.781 34.997 20.518 1.00 45.26 ATOM 502 CG LEU 69 48.781 34.997 22.848 1.00 46.33 ATOM 503 CD1 LEU 69 49.166 33.298 22.932 1.00 46.09 ATOM 505 C LEU 69 49.811 36.072 22.748 1.00 45.48 ATOM 505 C LEU 69 49.811 36.072 22.748 1.00 45.48 ATOM 507 N SER 70 45.228 34.758 20.351 1.00 45.75 ATOM 508 CA SER 70 44.177 35.528 19.697 1.00 44.78 ATOM 509 CB SER 70 44.275 33.899 19.844 1.00 44.25 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.72 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.72 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.72 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.52 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.52 ATOM 511 C SER 70 44.250 36.978 20.109 1.00 44.52 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.52 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.52 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.52 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.52 ATOM 510 C SER 70 44.250 36.978 20.109 1.00 44.52 ATOM 510 C SER 70 44.250 36.978 19.100 10.0 44.52 ATOM 510 C SER 70 44.250 36.978 19.100 10.0 49.53 ATOM 510 C SER 70 44.250 36.978 19.100 10.0 49.53 ATOM 510 C SER 70 44.250 36.978 19.100 10.0 49.53 ATOM 510 C SER 70 44.251 30.00 49.35 ATOM 510 C SER 70 44.251 30.00 49.35 ATOM 510 C SER 70 44.252 34.451 19.244 1.00 49.57 ATOM 510 C SER 70 44.252 34.451 19.244 1.00 49.59 ATOM 510 C SER 70 44.250 36.978 19.100 49.95 ATOM 510 C SER 70 44.250 36.978 19.100 49.95 ATOM 510 C	ATOM	490	CB	PHE	68	46.031			
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ATOM 526 OD2 ASP 72 38.168 41.777 21.331 1.00 50.11									
	MOTA	526	OD2	ASP	72	38.168	41.777	21.331	1.00 50.11

Figur 4

ATOM	527	С	ASP	72	40.819	42.962	19.258	1.00 48.98
ATOM	528	0	ASP	72	40.247	43.530	20.187	1.00 48.82
ATOM	529	N	LEU	73	41.312	43.613	18.214	1.00 49.73
MOTA	530	CA	LEU	73	41.193	45.060	18.117	1.00 51.48
MOTA	531	CB	LEU	73	42.199	45.603	17.096	1.00 50.80
MOTA	532	CG	LEU	73	42.160	47.096	16.774	1.00 50.07
ATOM	533	CD1	LEU	73	42.358	47.902	18.045	1.00 50.10
ATOM	534	CD2	LEU	73	43.223	47.421	15.738	1.00 49.97
ATOM	535	С	LEU	73	39.764	45.392	17.687	1.00 52.93
ATOM	536-	0	LEU	73	38.909	44.507	17.628	1.00 52.38
ATOM	537	N	GLY	74	39.504	46.665	17.401	1.00 54.88
ATOM	538	CA	GLY	74	38.177	47.068	16.983	1.00 56.88
ATOM	539	С	GLY	74	37.285	47.420	18.148	1.00 58.48
ATOM	540	0	GLY	74	36.476	48.348	18.071	1.00 58.31
ATOM	541	N	GLY	75	37.428	46.668	19.233	1.00 60.27
ATOM	542	CA	GLY	75	36.621	46.925	20.410	1.00 62.46
ATOM	543	С	GLY	75	37.020	48.230	21.074	1.00 63.75
ATOM	544	0	GLY	75	37.824	49.005	20.536	1.00 64.06
ATOM	545	N	THR	76	36.452	48.481	22.248	1.00 64.50
ATOM	546	CA	THR	76	36.759	49.697	22.991	1.00 65.42
ATOM	547	CB	THR	76	35.905	49.776	24.266	1.00 66.28
ATOM	548	OG1	THR	76	36.361	48.791	25.203	1.00 67.43
ATOM	549	CG2	THR	76	34.425	49.505	23.938	1.00 66.14
ATOM	550	C	THR	76	38.238	49.651	23.385	1.00 65.25
ATOM	551	0	THR	76	39.005	50.595	23.152	1.00 65.01
ATOM	552	N	ASN	77	38.622	48.528	23.980	1.00 64.74
ATOM	553	CA	ASN	77	39.987	48.309	24.412	1.00 64.17
ATOM	554	CB	ASN	77	40.015	47.966	25.903	1.00 65.44
ATOM	555	CG	ASN	77	39.346	49.027	26.765	1.00 66.47
ATOM	556	OD1	ASN	77	39.656	50.219	26.663	1.00 67.13
ATOM	557	ND2	ASN	77	38.431	48.596	27.629	1.00 66.65
MOTA	558	С	ASN	77	40.547	47.149	23.603	1.00 63.19
MOTA	559	0	ASN	77	39.795	46.303	23.120	1.00 62.58
MOTA	560	N	PHE	78	41.866	47.123	23.446	1.00 62.14
MOTA	561	CA	PHE	78	42.526	46.051	22.708	1.00 61.12
ATOM	562	CB	PHE	78	43.887	46.514	22.172	1.00 61.81
ATOM	563	CG	PHE	78	44.684	45.420	21.516	1.00 62.50
MOTA	564	CD1		78	44.347	44.956	20.245	1.00 62.81
MOTA	565		PHE	78	45.741	44.818	22.189	1.00 62.99
ATOM	566	CE1		78	45.051	43.899	19.655	1.00 62.72
ATOM	567		PHE	78	46.450	43.763	21.607	1.00 63.38
ATOM	568	CZ	PHE	78	46.103	43.301	20.336	1.00 63.01
ATOM	569	С	PHE	78	42.732	44.893	23.668	1.00 60.09
MOTA	570	0	PHE	78	43.065	45.100	24.834	1.00 60.08
ATOM	571	N	ARG	79	42.528	43.675	23.184	1.00 58.63
MOTA	572	CA	ARG	79	42.706	42.504	24.025	1.00 57.40
ATOM	573	CB	ARG	79	41.367	41.819	24.280	1.00 57.06
ATOM	574	CG	ARG	79	41.481	40.637	25.222	1.00 57.49
ATOM	575	CD	ARG	79	40.221	39.819	25.219	1.00 57.47
ATOM	576	NE	ARG	79	39.062	40.646	25.504	1.00 57.16
MOTA	577	CZ	ARG	79	37.818	40.266	25.267	1.00 57.69
ATOM	578		ARG	79	37.586	39.071	24.738	1.00 57.38
MOTA	579		ARG	79	36.812	41.080	25.555	1.00 58.45
ATOM	580	C	ARG	79	43.663	41.522	23.368	1.00 56.71
ATOM	581	0	ARG	79	43.926	41.619	22.170	1.00 57.24
ATOM	582	N	VAL	80	44.180	40.590	24.167	1.00 55.50
MOTA	583	CA	VAL	80	45.114	39.557	23.724	1.00 54.27
ATOM	584	CB	VAL	80	46.576	39.947	23.996	1.00 54.31
ATOM	585	CGI	VAL	80	47.491	38.779	23.674	1.00 54.49

Figur 4

ATOM	586	CG2	VAL	80	46.960	41.158	23.166	1.00 54.39
ATOM	587	С	VAL	80	44.806	38.327	24.555	1.00 54.04
ATOM	588	ō	VAL	80	44.517	38.447	25.738	1.00 53.31
ATOM	589	N	MSE	81	44.881	37.144	23.957	1.00 54.52
ATOM	590	CA	MSE	81	44.568	35.935	24.703	1.00 54.59
ATOM	591	CB	MSE	81	43.053	35.804	24.828	1.00 57.08
ATOM	592	CG	MSE	81	42.300	36.025	23,520	1.00 60.39
ATOM	593	SE	MSE	81	40.534	36.437	23.792	1.00 65.62
	594	CE	MSE	81	39.999	34.926	24.679	1.00 62.03
MOTA	595	C	MSE	81	45.142	34.645	24.146	1.00 53.56
MOTA	596	0	MSE	81	45.598	34.582	23.007	1.00 52.99
ATOM	597	N	LEU	82	45.096	33.611	24.978	1.00 52.63
ATOM				82	45.602	32.292	24.638	1.00 51.86
MOTA	598	CA	LEU		46.660	31.863	25.665	1.00 52.75
MOTA	599	CB	LEU	82 82	47.261	30.455	25.542	1.00 53.22
ATOM	600	CG	LEU	82	48.562	30.521	24.736	1.00 52.42
ATOM	601			82	47.523	29.882	26.937	1.00 53.00
MOTA	602		LEU			31.286	24.650	1.00 51.18
MOTA	603	С	LEU	82	44.461		25.632	1.00 51.20
ATOM	604	0	LEU	82	43.718	31.186	23.563	1.00 50.58
MOTA	605	N	VAL	83	44.333	30.535		1.00 50.00
ATOM	606	CA	VAL	- 83	43.292	29.522	23.448	1.00 49.63
MOTA	607	CB	VAL	83	42.274	29.887	22.362	1.00 49.26
ATOM	608		VAL	83	41.213	28.794	22.262	
ATOM	609		VAL	83	41.660	31.244	22.670	1.00 48.32
MOTA	610	С	VAL	83	43.914	28.187	23.080	
ATOM	611	0	VAL	83	44.759	28.122	22.192	1.00 50.93
ATOM	612	N	LYS	84	43.496	27.127	23.763	1.00 51.05
ATOM	613	CA	LYS	84	44.017	25.788	23.504	1.00 51.89
ATOM	614	CB	LYS	84	44.338	25.061	24.826	1.00 51.79
ATOM	615	CG	LYS	84	44.716	23.581	24.659	1.00 51.85
ATOM	616	CD	LYS	84	44.951	22.870	26.009	1.00 51.58
ATOM	617	CE	LYS	84	46.429	22.848	26.422	1.00 50.92
ATCM	618	NZ	LYS	84	47.041	24.198	26.592	1.00 50.33
MOTA	619	С	LYS	84	42.997	24.983	22.708	1.00 52.68
MOTA	620	0	LYS	84	42.115	24.327	23.282	1.00 53.00
ATOM	621	N	VAL	85	43.124	25.038	21.383	1.00 52.91
ATOM	622	CA	VAL	85	42.224	24.319	20.488	1.00 52.70
ATOM	623	CB	VAL	85	42.399	24.805	19.048	1.00 51.79
MOTA	624	CG:	l VAL	85	41.302	24.232	18.176	1.00 52.19
MOTA	625	CG:		85	42.389	26.319	19.017	1.00 51.59
ATOM	626	С	VAL	85	42.525	22.823	20.548	1.00 53.51
MOTA	627	0	VAL	85	43.637	22.389	20.243	1.00 53.87
ATOM	628	N	GLY	86	41.534	22.037	20.952	1.00 54.38
ATOM	629	CA	GLY	86	41.726	20.603	21.053	1.00 55.35
ATOM	630	C	GLY	86	40.901	19.810	20.060	1.00 56.21
MOTA	631	0	GLY	86	40.136	20370	19.278	1.00 55.63
MOTA	632	N	GLU	87	41.050	18.493	20.106	1.00 57.81
ATOM	633	CA	GLU	87	40,339	17.611	19.195	1.00 59.64
ATOM	634	CB	GLU	-87	41.290	16.529	18.673	
ATOM	635	CG	GLU	87	40.680		17.611	
MOTA	636	CD	GLU	87	40.215		16.423	1.00 63.21
MOTA	637	OE	1 GLU	87	41.072		15.644	
ATOM	638	OE	2 GLU	87	38.989	16.631	16.278	
ATOM	639		GLU	87	39.133	16.959	19.859	
ATOM	640		GLU	87	39.271	16.187	20.810	
ATOM	641		GLY	88	37.948	17.273	19.347	
ATOM	642			88	36.735		19.902	
ATOM	643		GLY	88	35.840		18.833	
ATOM	644		GLY	88	36.038		17.638	1.00 61.67

Figur 4

rıg	ur 4							
»mov	645	N	OT 17	89	34.845	15 262	10 274	1.00 62.79
ATOM ATOM	646	CA	GLU GLU	89	33.898	15.363 14.724	19.274 18.372	1.00 63.90
		CB	GLU	89	32.782	14.724	19.203	1.00 63.50
ATOM	647	CG		89				1.00 62.64
ATOM	648	CD	GLU	89	33.304 32.214	13.137	20.275	1.00 62.46
MOTA	649			89			21.203	1.00 62.46
ATOM	650	OE1	GLU	89	32.510 31.064	11.728	22.019	1.00 62.33
ATOM	651			89	33.312			1.00 65.16
MOTA	652	C	GLU			15.688	17.325	1.00 64.98
ATOM	653	0	GLU	89 90	32.975	16.837	17.634	1.00 66.03
MOTA	654	N	GLU		33.204	15.205	16.087	1.00 66.67
MOTA	655	CA	GLU	90	32.667	15.977	14.958	1.00 67.21
MOTA	656	CB	GLU	90	31.135	15.974	14.978	1.00 66.83
ATOM	657	CG	GLU	90	30.495	14.620	14.717	1.00 67.49
ATOM	658	CD	GLU	90	28.986	14.662	14.869	1.00 67.49
ATOM	659	OE1	GLU	90	28.308	15.273	14.009	1.00 66.84
ATOM	660		GLU	90	28.480	14.090	15.858	
ATOM	661	С	GLU	90 90	33.149	17.421	14.871	1.00 66.91
MOTA	662	0	GLU		32.623	18.212	14.080	1.00 66.74 1.00 67.05
ATOM	663	N	GLY	91	34.149	17.769	15.671	1.00 67.38
ATOM	664	CA	GLY	91	34.649	19.126	15.628	1.00 67.42
MOTA	665	C	GLY	91	36.036	19.339	16.201	1.00 68.24
MOTA	666	0	GLY	91	37.025	18.797	15.708	1.00 66.86
MOTA	667	N	GLN	92 92	36.094	20.154	17.246	1.00 65.88
ATOM	668	CA	GLN		37.335	20.492	17.929	1.00 65.93
ATOM	669	CB	GLN	92 92	38.395	20.968	16.924	1.00 66.24
ATOM	670	CG	GLN			22.215	16.159	1.00 66.57
MOTA	671	CD	GLN	92 92	38.564	22.236	14.750	1.00 66.37
ATOM ATOM	672 673		GLN	92	39.177	21.260	14.007	1.00 66.54
ATOM	674	C	GLN	92	36.999	21.605	18.920	1.00 65.21
ATOM	675	0	GLN	92	36.625	22.721	18.530	1.00 65.44
ATOM	676	N	TRP	93	37.111	21.278	20.204	1.00 63.62
ATOM	677	CA	TRP	93	36.820	22.227	21.261	1.00 61.51
MOTA	678	CB	TRP	93	36.859	21.540	22.626	1.00 62.77
ATOM	679	CG	TRP	93	38.050	20.641	22.857	1.00 63.86
ATOM	680	CD2		93	39.213	20.943	23.637	1.00 64.17
ATOM	681	CE2		93	40.026	19.787	23.645	1.00 64.21
ATOM	682	CE3	TRP	93	39.647	22.080	24.336	1.00 64.11
ATOM	683		TRP	93	38.206	19.349	22.424	1.00 63.84
ATOM	684	NE1		93	39.387	18.830	22.897	1.00 63.69
ATOM	685	CZ2	TRP	93	41.246	19.731	24.324	1.00 64.43
ATOM	686	CZ3	TRP	93	40.859	22.026	25.009	1.00 64.63
ATOM	687	CH2	TRP	93	41.645	20.857	24.999	1.00 64.71
ATOM	688	С	TRP	93	37.784	23.393	21.248	1.00 59.53
ATOM	689	0	TRP	93	38.733	23.420	20.474	1.00 59.18
ATOM	690	N	SER	94	37.521	24,366	22.106	1.00 57.94
ATOM	691	CA	SER	94	38.353	25.549	22.207	1.00 56.46
ATOM	692	CB	SER	94	37880	26.615	21.219	1.00 56.58
ATOM	693	OG	SER	94	36.504	26.899	21.412	1.00 56.78
MOTA	694	С	SER	94	38.185	26.050	23.624	1.00 55.56
ATOM	695	0	SER	94	37.142	25.822	24.237	1.00 55.36
ATOM	696	N	VAL	95	39.208	26.722	24.146	1.00 54.53
MOTA	697	CA	VAL	95	39.152	27.248	25.504	1.00 53.17
MOTA	698	CB	VAL	95	39.511	26.183	26.549	1.00 52.17
ATOM	699		L VAL	95	39.742	26.844	27.891	1.00 52.13
MOTA	700		VAL	95	38.396	25.172	26.666	1.00 51.73
MOTA	701	С	VAL	95	40.099	28.399	25.719	1.00 52.74
MOTA	702	0	VAL	95	41.268	28.315	25.357	1.00 53.14
MOTA	703	N	LYS	96	39.587	29.469	26.318	1.00 52.63

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Figur 4

FI	gur 4							
ATOM	704	CA	LYS	96	40.402	20 625		1.00 52.93
ATOM	705	CB	LYS	96	39.513	30.637	26.629	1.00 53.25
ATOM	706	CG	LYS	96	40.277	31.849	26.932	1.00 53.25
ATOM	707	CD	LYS	96	39.910	33.129	27.231	
ATOM	708	CE		96		33.706	28.595	1.00 54.80
ATOM	708	NZ	LYS	96	38.427	34.102	28.682	1.00 55.69
ATOM	710	C	LYS	96	38.027	35.162	27.696	1.00 55.59
					41.154	30.218	27.882	1.00 52.96
MOTA MOTA	711 712	O N	LYS	96 97	40.546	29.733	28.834	1.00 52.93
ATOM	713	CA	THR	97	42.470	30.384	27.886	1.00 53.38
MOTA	714	CB	THR	97	43.253	29.980	29.050	1.00 53.93
ATOM	715	OG1		97	44.238 43.512	28.850 27.736	28.684 28.151	1.00 53.99 1.00 52.99
MOTA	716	CG2		97	44.998	28.394	29.918	1.00 55.29
MOTA	717	C	THR	97	44.036	31.132	29.510	1.00 53.82
MOTA	718	Ö	THR	97	44.330	31.132	30.866	1.00 53.82
ATOM	719	N	LYS	98	44.373	32.117	28.848	1.00 53.85
MOTA	720	CA	LYS	98	45.115	33.276	29.315	1.00 54.60
ATOM	721	CB	LYS	98	46.627	33.096	29.087	1.00 55.51
ATOM	722	CG	LYS	98	47.220	31.809	29.652	1.00 56.78
ATOM	723	CD	LYS	98	47.074	31.733	31.162	1.00 58.23
ATOM	724	CE	LYS	98	47.553	30.389	31.713	1.00 58.82
ATOM	725	NZ	LYS	98	47.404	30.320	33.201	1.00 58.98
ATOM	726	C	LYS	98	44.644	34.479	28.518	1.00 54.54
ATOM	727	ō	LYS	98	44.323	34.360	27.329	1.00 54.79
ATOM	728	N	HIS	99	44.590	35.632	29.173	1.00 54.03
ATOM	729	CA	HIS	99	44.193	36.853	28.496	1.00 54.03
ATOM	730	CB	HIS	99	42.720	36.793	28.052	1.00 55.02
ATOM	731	CG	HIS	99	41.732	36.872	29.172	1.00 55.71
ATOM	732	CD2	HIS	99	40.682	37.704	29.373	1.00 35.66
MOTA	733	ND1	HIS	99	41.739	35.999	30.239	1.00 56.19
MOTA	734	CE1	HIS	99	40.736	36.288	31.049	1.00 56.30
ATOM	735		HIS	99	40.080	37.319	30.546	1.00 56.72
MOTA	736	C	HIS	99	44.445	38.082	29.351	1.00 53.46
MOTA	737	0	HIS	99	44.526	38.007	30.577	1.00 53.47
MOTA	738	N	GLN	100	44.583	39.214	28.683	1.00 52.94
MOTA	739	CA	GLN	100	44.841	40.468	29.349	1.00 53.34
ATOM	740	CB	GLN	100	46.354	40.649	29.513	1.00 53.39
ATOM	741	CG	GLN	100	46.790	42.001	30.055	1.00 54.26
MOTA	742	CD	GLN	100	46.168	42.345	31.394	1.00 54.43
MOTA	743	OE1		100	46.349	41.629	32.384	1.00 55.27
ATOM ATOM	744 745	NE2	GLN	100	45.433	43.452	31.432	1.00 53.60
ATOM	745	C	GLN	100	44.243	41.567	28.481	1.00 53.43
ATOM	747	O N	THR	100 101	44.416	41.569	27.260	1.00 53.75
ATOM	748	CA	THR	101	43.527 42.905	42.493	29.105 28.367	1.00 52.90 1.00 53.12
ATOM	749	CB	THR	101	41.495	43.576	28.894	1.00 52.52
ATOM	750	OG1		101	40.789	42.582	28.925	1.00 52.85
ATOM	751	CG2	THR	101	40.752	44.808	27.999	1.00 52.23
ATOM	752	C	THR	1-01	43.731	44.845	28.499	1.00 53.61
ATOM	753	ō	THR	101	44.285	45.108	29.563	1.00 53.95
ATOM	754	N	TYR	102	43.809	45.628	27.422	1.00 54.10
ATOM	755	CA	TYR	102	44.585	46.869	27.422	1.00 55.36
ATOM	756	CB	TYR	102	45.878	46.708	26.608	1.00 54.89
ATOM	757	CG	TYR	102	46.788	45.569	27.015	1.00 54.25
ATOM	758	CD1		102	46.382	44.241	26.888	1.00 54.08
ATOM	759	CE1	TYR	102	47.227	43.197	27.226	1.00 53.44
ATOM	760	CD2		102	48.069	45.822	27.497	1.00 53.79
ATOM	761	CE2		102	48.922	44.785	27.840	1.00 53.76
ATOM	762	CZ	TYR	102	48.498	43.475	27.701	1.00 53.85

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ATOM	763	OH	TYR	102	49.355	42.442	28.021	1.00 54.03
MOTA	764	C	TYR	102	43.813	48.041	26.822	1.00 56.65
MOTA	765	ō	TYR	102	43.173	47.899	25.781	1.00 56.91
ATOM	766	N	SER	103	43.891	49.203	27.462	1.00 58.50
ATOM	767	CA	SER	103	43.217	50.385	26.938	1.00 60.94
ATOM	768	CB	SER	103	42.997	51.411	28.049	1.00 61.09
ATOM	769	OG	SER	103	44.231	51.829	28.602	1.00 62.50
MOTA	770	С	SER	103	44.090	50.985	25.833	1.00 62.31
MOTA	771	0	SER	103	45.293	50.729	25.771	1.00 62.27
MOTA	772	N	ALA	104	43.487	51.783	24.960	1.00 64.47
MOTA	773	CA	ALA	104	44.226	52.386	23.856	1.00 67.01
MOTA	774	CB	ALA	104	43.516	52.093	22.526	1.00 67.01
ATOM	775	C	ALA	104	44.410	53.888	24.025	1.00 68.66
ATOM	776	0	ALA	104	43.458	54.658	23.902	1.00 69.01
ATOM	777	N	PRO	105	45.648	54.327	24.305	1.00 70.09
ATOM	778	CD	PRO	105	46.878	53.522	24.397	1.00 70.06
ATOM	779	CA	PRO	105	45.946	55.751	24.485	1.00 71.25
ATOM	780	CB	PRO	105	47.443	55.748	24.783	1.00 70.79
MOTA	781	CG	PRO	105	47.929	54.535	24.046	1.00 70.54
ATOM	782	С	PRO	105	45.592	56.586	23.251	1.00 72.81
ATOM	783	0	PRO	105	45.837	56.170	22.117	1.00 73.09
MOTA	784	N	GLU	106	45.012	57.762	23.479	1.00 74.39
ATOM	785	CA	GLU	106	44.619	58.652	22.391	1.00 76.25
ATOM	786	CB	GLU	106	43.991	59.921	22.950	1.00 76.77
ATOM	787	CG	GLU	106	42.702	59.673	23.680	1.00 78.35
ATOM	788	CD	GLU	106	42.397	60.775	24.657	1.00 79.28
ATOM	789	OE1	GLU	106	42.239	61.934	24.214	1.00 79.74
ATOM	790	OE2	GLU	106	42.326	60.478	25.871	1.00 80.03
ATOM	791	C	GLU	106	45.784	59.028	21.494	1.00 77.33
ATOM	792	0	GLU	106	45.600	59.262	20.300	1.00 77.48
ATOM	793	N	ASP	107	46.980	59.104	22.068	1.00 78.72
ATOM	794	CA	ASP	107	48.161	59.440	21.284	1.00 80.10
MOTA	795	CB	ASP	107	49.431	59.316	22.134	1.00 80.44
ATOM	796	CG	ASP	107	49.965	57.889	22.185	1.00 81.03
ATOM	797		ASP	107	49.198	56.976	22.569	1.00 81.42
ATOM	798		ASP	107	51.151	57.682	21.839	1.00 80.86
ATOM	799	С	ASP	107	48.212	58.424	20.151	1.00 80.92
ATOM	800	0	ASP	107	48.724	58.703	19.065	1.00 81.29
ATOM	801	N	ALA	108	47.67C	57.241	20.428	1.00 81.68
MOTA	802	CA	ALA	108	47.628	56.151	19.463	1.00 82.45
ATOM	803	CB	ALA	108	47.605	54.813	20.200	1.00 82.45
ATOM	804	C	ALA	108	46.406	56.275	18.553	1.00 82.91
ATOM	805	0	ALA	108	46.536	56.351	17.331	1.00 82.98
ATOM	806	N	MSE	109	45.221	56.303	19.157	1.00 83.41
ATOM	807	CA	MSE	109	43.974	56.414	18.407	1.00 83.78
ATOM	808	CB	MSE	109	42.787	56.519	19.368	1.00 85.45 1.00 87.01
ATOM ATOM	809 810	CG SE	MSE MSE	109 109	41.581	55.678	18.972	1.00 87.01
ATOM	811	CE	MSE	109	42.665	53.898 53.581	19.096 17.453	1.00 90.12
ATOM	812		MSE	109				1.00 83.17
ATOM	813	c o	MSE	109	43.992 43.235	57.633 57.710	17.494 16.527	1.00 83.19
ATOM	814	N	THR	110	44.854	58.590	17.820	1.00 82.51
ATOM	815	CA	THR	110	44.054	59.815	17.040	1.00 82.00
ATOM	815	CB	THR	110	44.986	61.022	17.040	1.00 82.00
ATOM	817	OG1		110	44.302	61.103	18.986	1.00 83.00
ATOM	818	CG2		110	45.283	62.313	17.142	1.00 82.69
ATOM	819	C	THR	110	46.150	59.640	16.082	1.00 81.25
ATOM	820	ō	THR	110	46.137	60.123	14.949	1.00 80.95
ATOM	821	N	GLY	111	47.168	58.933	16.559	1.00 80.84
11100	021	14	901	111	47.100	20.23	10.555	2.00 00.04

Figur 4

ATOM	822	CA	GLY	111	48.358	58.691	15.768	1.00 80.12
ATOM	823	С	GLY	111	48.121	57.986	14.450	1.00 79.53
ATOM	824	0	GLY	111	47.018	57.531	14.148	1.00 79.54
ATOM	825	N	THR	112	49.181	57.904	13.658	1.00 78.87
MOTA	826	CA	THR	112	49.129	57.254	12.360	1.00 78.09
ATOM	827	CB	THR	112	50.427	57.553	11.561	1.00 78.67
ATOM	828		THR	112	50.329	57.001	10.240	1.00 79.18
MOTA	829		THR	112	51.644	56.956	12.279	1.00 78.48
ATOM	830	C	THR	112	48.992	55.748	12.579	1.00 77.09
	831	0	THR	112	49.231	55.254	13.685	1.00 76.48
ATOM				113			11.529	1.00 76.26
ATOM	832	N	ALA		48.601	55.027		
MOTA	833	CA	ALA	113	48.443	53.573	11.603	1.00 75.60
MOTA	834	CB	ALA	113	48.184	53.001	10.208	1.00 76.00
MOTA	835	С	ALA	113	49.711	52.965	12.191	1.00 74.65
ATOM	836	0	ALA	113	49.665	52.006	12.968	1.00 74.58
ATOM	837	N	GLU	114	50.845	53.538	11.803	1.00 73.24
ATOM	838	CA	GLU	114	52.139	53.088	12.288	1.00 71.57
ATOM	839	CB	GLU	114	53.246	53.971	11.700	1.00 72.34
ATOM	840	ÇG	GLU	114	53.130	54.167	10.188	1.00 71.64
MOTA	841	CD	GLU	114	53.325	52.877	9.401	1.00 72.49
ATOM	842	OE1	GLU	114	53.192	51.781	9.994	1.00 72.24
ATOM	843	OE2	GLU	114	53.600	52.960	8.183	1.00 71.83
ATOM	844	С	GLU	114	52.085	53.233	13.801	1.00 70.37
ATOM	845	0	GLU	114	52.297	52.266	14.537	1.00 69.92
ATOM	846	N	MET	115	51.778	54.450	14.246	1.00 68.75
ATOM	847	CA	MET	115	51.657	54.760	15.669	1.00 66.97
ATOM	848	CB	MET	115	51.013	56.140	15.866	1.00 67.15
ATOM	849	CG	MET	115	51.999	57.277	16.040	1.00 66.94
MOTA	850	SD	MET	115	53.203	56.869	17.320	1.00 67.61
ATOM	851	CE	MET	115	52.137	56.732	18.788	1.00 66.65
ATOM	852	c	MET	115	50.799	53.718	16.374	1.00 65.81
MOTA	853	Ö	MET	115	51.266	53.010	17.275	1.00 65.94
ATOM	854	N	LEU	116	49.542	53.635	15.940	1.00 63.70
ATOM	855	CA	LEU	116	48.561	52.711	16.504	1.00 61.63
MOTA	856	CB	LEU	116	47.287	52.720	15.650	1.00 60.89
ATOM	857	CG	LEU	116	45.948	52.726	16.205	1.00 59.42
ATOM	858		LEU	116	44.953	52.182	15.051	1.00 58.84
MOTA	859		LEU	116	46.081	50.858	16.847	1.00 58.86
ATOM	860	C	LEU	116	49.083	51.285	16.613	1.00 60.35
ATOM	861	0	LEU	116	48.977	50.665	17.667	1.00 60.48
ATOM	862	N	PHE	117	49.641	50.756	15.531	1.00 59.14
		CA	PHE	117				1.00 58.14
ATOM	863	CB		117	50.138	49.391	15.580 14.173	1.00 57.03
ATOM	864		PHE		50.298	48.819		1.00 56.22
ATOM	865	CG	PHE	117	49.055	48.144	13.669	
ATOM	866	CD1		117	48.005	48.889	13.143	
ATOM	867	CD2		117	48.909	46.763	13.783	1.00 55.59
MOTA	868	CE1		117	46.830	48.270	12.741	1.00 55.25
ATOM	869	CE2		117	47.736	46.134	13.384	1.00 55.20
ATOM	870	CZ	PHE	117	46.695	46.887	12.862	1.00 55.23
ATOM	871	C	PHE	117	51.415	49.204	16.382	1.00 57.89
ATOM	872	0	PHE	117	51.799	48.073	16.690	1.00 57.80
MOTA	873	N	ALA	118	52.078	50.303	16.725	1.00 57.35
MOTA	874	CA	ALA	118	53.275	50.193	17.537	1.00 56.79
MOTA	875	CB	ALA	118	54.004	51.533	17.594	1.00 56.42
MOTA	876	С	ALA	118	52.747	49.792	18.922	1.00 56.46
MOTA	877	0	ALA	118	53.220	48.829	19.536	1.00 56.68
MOTA	878	N	ALA	119	51.733	50.515	19.391	1.00 55.57
ATOM	879	CA	ALA	119	51.142	50.226	20.693	1.00 55.05
ATOM	880	CB	ALA	119	49.931	51.135	20.952	1.00 53.91

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ATOM	881	С	ALA	119	50.719	48.769	20.763	1.00 54.96
ATOM	882	0	ALA	119	51.090	48.052	21.698	1.00 54.94
MOTA	883	N	ILE	120	49.948	48.338	19.763	1.00 55.10
ATOM	884	CA	ILE	120	49.443	46.969	19.715	1.00 55.51
MOTA	885	CB	ILE	120	48.679	46.679	18.397	1.00 54.45
MOTA	886	CG2	ILE	120	47.922	45.363	18.525	1.00 53.30
ATOM	887	CG1	ILE	120	47.688	47.808	18.089	1.00 53.32
MOTA	888	CD1	ILE	120	46.871	47.581	16.820	1.00 51.70
ATOM	889	С	ILE	120	50.575	45.957	19.846	1.00 56.57
ATOM	890	0	ILE	120	50.477	45.006	20.632	1.00 56.52
MOTA	891	N	SER	121	51.645	46.169	19.076	1.00 57.78
ATOM	892	CA	SER	121	52.814	45.284	19.093	1.00 58.54
MOTA	893	CB	SER	121	53.844	45.730	18.045	1.00 58.96
MOTA	894	OG	SER	121	53.377	45.507	16.720	1.00 59.32
MOTA	895	C	SER	121	53.457	45.280	20.473	1.00 58.74
ATOM	896	0	SER	121	54.007	44.265	20.918	1.00 57.56
MOTA	897	N	GLU	122	53.379	46.422	21.151	1.00 59.50
MOTA	898	CA	GLU	122	53.947	46.529	22.484	1.00 60.44
MOTA	899	CB	GLU	122	54.003	47.986	22.941	1.00 60.60
MOTA	900	CG	GLU	122	55.104	48.241	23.952	1.00 60.45
MOTA	901	CD	GLU	122	54.706	49.252	25.003	1.00 61.76
MOTA	902	OE1	GLU	122	54.152	50.312	24.630	1.00 61.92
MOTA	903	OE2	GLU	122	54.950	48.986	26.202	1.00 62.20
MOTA	904	C	GLU	122	53.091	45.725	23.452	1.00 60.63
MOTA	905	0	GLU	122	53.565	44.761	24.048	1.00 60.82
MOTA	906	N	CYS	123	51.831	46.120	23.605	1.00 60.96
ATOM	907	CA	CYS	123	50.936	45.410	24.510	1.00 61.79
MOTA	908	CB	CYS	123	49.481	45.840	24.278	1.00 61.63
MOTA	909	SG	CYS	123	49.191	47.636	24.439	1.00 62.83
MOTA	910	C	CYS	123	51.107	43.922	24.233	1.00 61.90
MOTA	911	0	CYS	123	51.028	43.095	25.147	1.00 61.89
MOTA	912	N	ILE	124	51.350	43.588	22.966	1.00 62.36
ATOM	913	CA	IĻE	124	51.561	42.197	22.588	1.00 62.79
MOTA	914	CB	ILE	124	52.033	42.061	21.109	1.00 62.52
MOTA	915	CG2		124	52.618	40.676	20.877	1.00 61.07
MOTA	916	CG1		124	50.866	42.280	20.138	1.00 61.53
MOTA	917	CD1		124	50.016	41.038	19.888	1.00 61.77
ATOM	918	C	ILE	124	52.673	41.706	23.499	1.00 62.76
MOTA	919	0	ILE	124	52.475	40.807	24.320	1.00 62.23
ATOM	920	N	SER	125	53.839	42.327	23.347	1.00 63.43
ATOM	921	CA	SER	125	55.020	42.002	24.138	1.00 64.63
ATOM	922	CB	SER	125	56.062	43.117	23.986	1.00 65.05
MOTA	923	OG	SER	125 125	57.324	42.745	24.523	1.00 67.01
MOTA	924 925	C	SER	125	54.646	41.840	25.610	1.00 64.32
ATOM			SER		54.886	40.794	26.219	
ATOM ATOM	926 927	N CA	ASP ASP	126 126	54.047 53.626	42.884	26.169	1.00 64.43 1.00 64.86
ATOM	928	CB	ASP	126	52.660	42.894	27.562 27.788	1.00 64.85
ATOM	929	CG		126			29.253	1.00 65.38
ATOM	930	OD1	ASP ASP	126	52.390 51.952	44.323	29.255	1.00 65.74
ATOM	931	OD2		126	52.613		29.706	1.00 65.92
ATOM	932	C	ASP	126	52.968	45.467 41.572	27.980	1.00 64.65
	933	o		126				1.00 64.28
ATOM ATOM	934	N	ASP PHE	125	53.424 51.902	40.918	28.924 27.274	1.00 64.26
ATOM	935	CA	PHE	127	51.902	39.948	27.565	1.00 65.21
ATOM	935	CB	PHE	127	50.145	39.948	26.468	1.00 64.22
	936	CG	PHE	127			26.525	1.00 64.22
ATOM ATOM	937		PHE	127	49.569 48.774	38.258 37.857	26.525	1.00 63.64
	939			127	49.830	37.343	25.512	1.00 63.42
MOTA	239	CDZ	PHE	261	47.030	37.343	23.312	2.00 05.42

Figur 4

MOTA	940	CE1	PHE	127	48.247	36.564	27.652	1.00 63.40
ATOM	941	CE2	PHE	127	49.308	36.051	25.560	1.00 63.55
ATOM	942	CZ	PHE	127	48.516	35.661	26.632	1.00 63.49
ATOM	943	C	PHE	127	52.154	38.791	27.631	1.00 65.83
MOTA	944	ō	PHE	127	52.195	38.030	28.600	1.00 65.71
MOTA	945	N	LEU	128	52.931	38.684	26.562	1.00 66.57
MOTA	946	CA	LEU	128	53.942	37.656	26.387	1.00 67.52
ATOM	947	CB	LEU	128	54.773	38.022	25.166	1.00 67.64
ATOM	948	CG	LEU	128	53.926	38.452	23.969	1.00 67.42
ATOM	949		LEU	128	54.819	39.108	22.941	1.00 67.90
ATOM	950		LEU	128	53.195	37.251	23.387	1.00 67.65
ATOM	951	C	LEU	128	54.850	37.502	27.609	1.00 68.09
ATOM	952	Ó	LEU	128	54.829	36.468	28.285	1.00 67.92
ATOM	953	N	ASP	129	55.654	38.530	27.878	1.00 68.62
ATOM	954	CA	ASP	129	56.565	38.514	29.018	1.00 69.22
MOTA	955	CB	ASP	129	57.135	39.907	29.287	1.00 68.93
ATOM	956	CG	ASP	129	58.115	40.342	28.239	1.00 68.90
ATOM	957	OD1	ASP	129	59.100	39.606	28.011	1.00 69.12
ATOM	958	OD2	ASP	129	57.900	41.423	27.650	1.00 69.22
ATOM	959	С	ASP	129	55.843	38.059	30.267	1.00 69.59
ATOM	960	0	ASP	129	56.063	36.956	30.761	1.00 69.41
ATOM	961	N	LYS	130	54.973	38.940	30.753	1.00 70.10
ATOM	962	CA	LYS	130	54.190	38.733	31.958	1.00 70.67
ATOM	963	CB	LYS	130	53.285	39.946	32.159	1.00 70.80
ATOM	964	CG	LYS	130	54.076	41.252	32.052	1.00 70.54
MOTA	965	CD	LYS	130	53.218	42.479	32.266	1.00 70.22
ATOM	966	CE	LYS	130	54.021	43.746	32.011	1.00 70.07
ATOM	967	NZ	LYS	130	53.204	44.977	32.195	1.00 69.69
MOTA	968	C	LYS	130	53.394	37.441	31.982	1.00 71.17
ATOM	969	0	LYS	130	52.381	37.331	32.673	1.00 70.99
MOTA	970	Ν.	HIS	131	53.883	36.468	31.221	1.00 72.01
ATOM	971	CA	HIS	131	53.301	35.139	31.125	1.00 73.44
MOTA	972	CB	HIS	131	52.313	35.065	29.965	1.00 73.00
MOTA	973	CG	HIS	131	50.881	35.076	30.397	1.00 72.93
MOTA	974		HIS	131	49.960	34.085	30.454	1.00 72.73
ATOM	975		HIS	131	50.256	36.210	30.869	1.00 72.87
ATOM	976		HIS	131	49.010	35.917	31.196	1.00 73.01
MOTA	977		HIS	131	48.806	34.634	30.954	1.00 73.04
ATOM	978	С	HIS	131	54.424	34.124	30.908	1.00 74.61
ATOM	979	0	HIS	131	54.419	33.049	31.514	1.00 74.70
ATOM	980	N	GLN	132	55.374	34.502	30.046	1.00 76.14
ATOM	981	CA	GLN	132	56.566	33.727	29.658	1.00 77.30
MOTA	982	CB	GLN	132	56.536	32.293	30.218	1.00 77.68
ATOM	983	CG	GLN	132	55.424	31.387	29.676	1.00 78.41
ATOM	984	CD	GLN	132	55.823	30.611	28.436	1.00 78.88
ATOM	985	OE1		132	56.016	31,179	27.356	1.00 78.50
ATOM	986	NE2		132	55.951	29.294	28.587	1.00 79.41
ATOM	987	С	GLN	132	56-673	33.682	28.134	1.00 77.86
MOTA	988	0	GLN	132	57.769	33.638	27.574	1.00 77.91 1.00 78.39
ATOM	989	N	MSE	133	55.520	33.703	27.472	
ATOM	990 991	CA	MSE	133	55.450	33.662	26.017	1.00 78.88 1.00 80.96
ATOM				133	53.989	33.684	25.551	1.00 80.96
ATOM	992 993	CG SE	MSE	133	53.278	32.347	25.586 26.846	1.00 83.34
ATOM ATOM	994	CE	MSE	133 133	51.991 52.168	32.273	25.845	1.00 84.33
ATOM	995	CE	MSE	133	56.174	34.812	25.333	1.00 77.90
ATOM	995	0	MSE	133	55.552	35.548	24.567	1.00 77.90
ATOM	996	N	LYS	134	57.470	34.973	25.587	1.00 75.97
ATOM	998	CA	LYS	134	58.225	36.053	24.949	1.00 73.96
MION	220	CA	115	174	50.225	30.053	44.949	1.00 /3.90

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Figur 4

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MOTA	999	СВ	LYS	134	58.976	36.879	25.997	1.00 73.14
ATOM	1000	CG	LYS	134	59.676	38.125	25.454	1.00 72.28
ATOM	1001	CD	LYS	134	58.697	39.250	25.434	1.00 70.99
ATOM	1002	CE	LYS	134	59.415	40.586	24.935	1.00 70.06
ATOM	1003	NZ	LYS	134	60.234	40.640	23.687	1.00 69.46
ATOM	1004	C	LYS	134	59.211	35.443	23.964	1.00 72.94
ATOM	1005	ō	LYS	134	59.727	36.123	23.077	1.00 72.63
MOTA	1006	N	HIS	135	59.457	34.148	24.132	1.00 72.28
ATOM	1007	CA	HIS	135	60.377	33.411	23.275	1.00 71.52
ATOM	1008	CB	HIS	135	61.359	32.584	24.119	1.00 71.15
ATOM	1009	CG	HIS	135	60.719	31.448	24.859	1.00 70.88
ATCM	1010		HIS	135	60.908	30.109	24.773	1.00 70.87
MOTA	1011	ND1	HIS	135	59.750	31.635	25.822	1.00 70.81
ATOM	1012	CE1	HIS	135	59.370	30.462	26.298	1.00 70.56
ATOM	1013	NE2	HIS	135	60.057	29.519	25.678	1.00 70.85
MOTA	1014	C	HIS	135	59.584	32.482	22.365	1.00 71.26
ATOM	1015	0	HIS	135	60.152	31.818	21.499	1.00 71.53
ATOM	1016	N	LYS	136	58.272	32.434	22.574	1.00 70.85
ATOM	1017	CA	LYS	136	57.393	31.590	21.766	1.00 70.33
ATOM	1018	CB	LYS	136	56.077	31.329	22.508	1.00 69.64
ATOM	1019	CG	LYS	136	56.225	30.694	23.886	1.00 68.45
ATCM	1020	CD	LYS	136	56.740	29.271	23.783	1.00 68.01
ATOM	1021	CE	LYS	136	56.698	28.560	25.128	1.00 67.56
ATOM	1022	NZ	LYS	136	55.303	28.356	25.623	1.00 66.87
ATOM	1023	C	LYS	136	57.088	32.296	20.443	1.00 70.46
ATOM	1024	0	LYS	136	57.100	33.530	20.371	1.00 70.94
ATOM	1025	N	LYS	137	56.828	31.519	19.396	1.00 70.16
ATOM ATOM	1026 1027	CA	LYS	137 137	56.505	32.096	18.096	1.00 69.80
ATOM	1027	CG	LYS	137	57.505	31.642	17.023	1.00 71.09
ATOM	1029	CD	LYS	137	57.602 58.567	30.132	16.801	1.00 71.73 1.00 72.44
ATOM	1030	CE	LYS	137	58.915	28.363	15.654 15.545	1.00 72.44
ATOM	1031	NZ	LYS	137	59.919	28.136	14.463	1.00 72.59
ATON	1032	C	LYS	137	55.097	31.685	17.702	1.00 68.73
ATOM	1033	ō	LYS	137	54.799	31.476	16.524	1.00 69.92
ATOM	1034	N	LEU	138	54.243	31.579	18.716	1.00 66.57
ATOM	1035	CA	LEU	138	52.841	31.193	18.586	1.00 63.82
ATOM	1036	CB	LEU	138	52.057	31.788	19.748	1.00 63.11
ATOM	1037	CG	LEU	138	52.364	31.145	21.092	1.00 62.89
ATOM	1038	CD1	LEU	138	51.924	32.068	22.220	1.00 62.68
ATOM	1039	CD2	LEU	138	51.669	29.786	21.150	1.00 61.80
MOTA	1040	C	LEU	138	52.114	31.553	17.294	1.00 62.26
MOTA	1041	0	LEU	138	52.416	32.566	16.647	1.00 62.54
ATOM	1042	N	PRO	139	51.149	30.708	16.894	1.00 60.11
ATOM	1043	CD	PRO	139	50.841	29.394	17.489	1.00 59.82
ATOM	1044	CA	PRO	139	50.356	30.937	15.682	1.00 57.91
ATOM	1045	CB	PRO	139	49.761	29.564	15.398	1.00 58.05
ATOM ATOM	1046	CG	PRO	139	49.573	28.999	16.772	1.00 59.12
ATOM	1047 1048	C O	PRO	139 139	49.302	31.968	16.101	1.00 55.89
ATOM		N			.48.469	31.693	16.973	1.00 55.71
ATOM	1049 1050	CA	LEU	140 140	49.358 48.440	33.154	15.501	1.00 53.40 1.00 50.78
ATOM	1050	CB	LEU	140	48.440	34.237	15.850	1.00 50.78
ATOM	1052	CG	LEU	140	49.193	35.576 36.893	15.834	1.00 49.87
ATOM	1052	CD1	LEU	140	49.414	37.933	16.646	1.00 48.17
ATOM	1054	CD2	LEU	140	47.825	37.389	14.801	1.00 48.88
ATOM	1055	C	LEU	140	47.169	34.359	15.018	1.00 49.13
ATOM	1056	ō	LEU	140	47.211	34.368	13.785	1.00 49.12
MOTA	1057	N	GLY	141	46.040	34.441	15.722	1.00 46.93

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ATOM	1058	CA	GLY	141	44.743	34.613	15.086	1.00 43.70
ATOM	1059	C	GLY	141	44.324	36.041	15.402	1.00 41.11
ATOM	1060	ō	GLY	141	44.277	36.414	16.569	1.00 41.46
MOTA	1061	N	PHE	142	44.018	36.842	14.388	1.00 38.27
ATOM	1062	CA	PHE	142	43.659	38.232	14.629	1.00 36.42
ATOM	1063	CB	PHE	142	44.648	39.118	13.882	1.00 34.58
MOTA	1064	CG	PHE	142	44.403	40.593	14.037	1.00 33.28
MOTA	1065	CD1	PHE	142	43.941	41.124	15.229	1.00 32.86
MOTA	1066	CD2	PHE	142	44.702	41.465	12.992	1.00 32.75
MOTA	1067	CE1	PHE	142	43.784	42.505	15.375	1.00 32.95
ATOM	1068		PHE	142	44.551	42.845	13.125	1.00 31.57
ATOM	1069	CZ	PHE	142	44.094	43.365	14.313	1.00 32.24
MOTA	1070	С	PHE	142	42.224	38.652	14.300	1.00 36.83
ATOM	1071	0	PHE	142	41.843	38.801	13.124	1.00 36.76
ATOM	1072	N	THR	143	41.423	38.848	15.347	1.00 35.96
ATOM	1073	CA	THR	143	40.047	39.288	15.156	1.00 34.35
ATOM	1074	CB	THR	143	39.179	38.997	16.373	1.00 33.98
ATOM	1075		THR	143	38.947	37.586	16.472	1.00 33.45
ATOM ATOM	1076 1077	CG2	THR	143 143	37.854	39.750	16.255	1.00 33.35
ATOM	1078	0	THR	143	40.081	40.793	14.964	1.00 33.92
ATOM	1078	N	PHE	144	40.190 40.009	41.544	15.928 13.716	1.00 34.30
ATOM	1080	CA	PHE	144	40.009	42.649	13.716	1.00 31.69
ATOM	1081	CB	PHE	144	40.891	42.842	12.132	1.00 29.18
ATOM	1082	CG	PHE	144	41.189	44.264	11.807	1.00 26.95
ATOM	1083		PHE	144	41.727	45.108	12.763	1.00 25.21
MOTA	1084	CD2		144	40.956	44.755	10.533	1.00 25.39
MOTA	1085	CE1		144	42.026	46.428	12.450	1.00 26.79
ATOM	1086	CE2	PHE	144	41.250	46.070	10.212	1.00 25.46
ATOM	1087	CZ	PHE	144	41.785	46.910	11.167	1.00 25.80
ATOM	1088	C	PHE	144	38.562	42.981	13.112	1.00 32.02
MOTA	1089	0	PHE	144	37.929	42.280	12.333	1.00 33.96
MOTA	1090	N	SER	145	38.025	44.027	13.744	1.00 32.29
ATOM	1091	CA	SER	145	36.602	44.387	13.600	1.00 31.56
ATOM	1092	CB	SER	145	35.993	44.689	14.968	1.00 31.79
ATOM	1093	OG	SER	145	35.997	43.539	15.790	1.00 33.15
ATOM	1094	С	SER	145	36.271	45.546	12.679	1.00 30.95
ATOM	1095	0	SER	145	35.601	46.508	13.082	1.00 30.63
ATOM ATOM	1096 1097	N CA	PHE	146 146	36.723 36.452	45.456	11.439	1.00 30.27 1.00 29.49
ATOM	1098	CB	PHE	146	37.573	46.513 47.541	10.489	1.00 29.49
ATOM	1099	CG	PHE	146	37.848	48.054	11.908	1.00 27.96
ATOM	1100		PHE	146	38.654	47.336	12.775	1.00 28.87
ATOM	1101		PHE	146	37.245	49.221	12.359	1.00 27.88
ATOM	1102		PHE	146	38.852	47.777	14.078	1.00 29.72
ATOM	1103	CE2		146	37.434	49,670	13.659	1.00 26.92
MOTA	1104	CZ	PHE	146	38.232	48.955	14.520	1.00 28.49
ATOM	1105	C	PHE	146	36.318	45.937	9.093	1.00 29.49
ATOM	1106	0	PHE	146	36.668	44.778	8.846	1.00 29.56
ATOM	1107	N	PRO	147	35.805	46.738	8.152	1.00 29.02
ATOM	1108	CD	PRO	147	35.452	48.167	8.211	1.00 28.09
ATOM	1109	CA	PRO	147	35.662	46.212	6.798	1.00 30.12
ATOM	1110	CB	PRO	147	34.852	47.309	6.099	1.00 28.65
ATOM	1111	CG	PRO	147	35.377	48.540	6.749	1.00 28.13
ATOM	1112	C	PRO	147	37.047	45.969	6.179	1.00 30.89
ATOM	1113	0	PRO	147	37.938	46.821	6.263	1.00 32.17
ATOM	1114	N	VAL	148	37.221	44.807	5.557	1.00 31.62
ATOM	1115	CA	VAL	148	38.499	44.453	4.957	1.00 32.00
MOTA	1116	CB	VAL	148	39.399	43.733	6.002	1.00 32.44

Figur 4

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ATOM	1117	CG1	WAT.	148	40.471	42.940	5.311	1.00 33.36
ATOM	1118	CG2		148	40.035	44.758	6.934	1.00 32.04
ATOM	1119	C	VAL	148	38.351	43.557	3.733	1.00 31.54
ATOM	1120	ō	VAL	148	37.937	42.402	3.858	1.00 30.91
ATOM	1121	N	ALA	149	38.688	44.091	2.560	1.00 31.65
ATOM	1122	CA	ALA	149	38.610	43.316	1.324	1.00 32.33
ATOM	1123	CB	ALA	149	38.834	44.213	0.120	1.00 32.33
ATOM	1124	C	ALA	149	39.723	44.213	1.428	1.00 31.15
ATOM	1125	0	ALA	149	40.882		1.428	1.00 35.59
ATOM	1126	N	HIS	150	39.387	42.653	1.535	1.00 33.33
	1127	CA	HIS	150		41.008		1.00 33.73
MOTA	1128	CB	HIS	150	40.410 39.868	39.980	1.666	1.00 33.88
ATOM	1129		HIS	150		38.780		1.00 34.82
MOTA	1130	CG	HIS	150	39.879	38.961	3.933	1.00 35.56
	1131		HIS	150	40.344	38.162	4.921	1.00 36.45
MOTA			HIS	150	39.329	40.061	4.555	1.00 36.45
ATOM	1132				39.454	39.930	5.865	
MOTA	1133		HIS	150	40.067	38.786	6.114	1.00 36.38
ATOM	1134	С	HIS	150	40.960	39.442	0.353	1.00 34.39
ATOM	1135	0	HIS	150	40.245	39.364	-0.655	1.00 34.56
ATOM	1136	N	ALA	151	42.239	39.068	0.380	1.00 34.73
ATOM	1137	CA	ALA	151	42.898	38.440	-0.762	1.00 34.53
ATOM	1138	CB	ALA	151	44.334	38.949	-0.919	1.00 34.86
ATOM	1139	C	ALA	151	42.894	36.968	-0.338	1.00 34.46
MOTA	1140	0	ALA	151	42.734	36.065	-1.161	1.00 34.16
ATOM	1141	N	ASP	152	43.050	36.754	0.970	1.00 34.36
ATOM	1142	CA	ASP	152	43.045	35.422	1.562	1.00 35.45
ATOM	1143	CB	ASP	152	44.335	34.687	1.214	1.00 37.69
ATOM	1144	CG	ASP	152	44.233	33.185	1.431	1.00 40.20
ATOM	1145		ASP	152	43.219	32.717	2.007	1.00 40.73
ATOM	1146		ASP	152	45.177	32.464	1.018	1.00 42.29
ATOM	1147	C 0	ASP	152	42.901	35.549	3.088	1.00 35.53
MOTA	1148 1149	N	ASP	152 153	43.048	36.642	3.642	1.00 35.08
				153	42.627	34.433	3.762	1.00 35.49 1.00 35.75
ATOM ATOM	1150 1151	CA	ILE	153	42.436	34.427	5.213 5.754	1.00 35.75
ATOM	1152		ILE	153	42.258	32.984	5.734	1.00 34.16
ATOM	1152	CG1		153	41.593	32.316	7.130	1.00 34.16
ATOM	1154		ILE	153	40.225	33.697	7.131	1.00 36.43
ATOM	1155	C	ILE	153	43.571	35.079	6.011	1.00 36.77
ATOM	1156	o	ILE	153	43.450	35.079	7.229	1.00 36.40
ATOM.	1157	N	ASP	154	44.665	35.411	5.332	1.00 37.10
ATOM	1158	CA	ASP	154	45.815	36.003	6.000	1.00 37.27
MOTA	1159	CB	ASP	154	46.982	35.013	5.991	1.00 38.98
ATOM	1160	CG	ASP	154	47.795	35.013	4.703	1.00 41.58
ATOM	1161		ASP	154	47.215	34.890	3,605	1.00 42.46
ATOM	1162		ASP	154	49.022	35.331	4.789	1.00 42.65
ATOM	1163	C	ASP	154	46.233	37.287	5.307	1.00 36.74
ATOM	1164	ō	ASP	154	47.360	37.751	5.471	1.00 37.07
ATOM	1165	N	ALA	1:55	45.328	37.865	4.531	1.00 35.91
ATOM	1166	CA	ALA	155	45.650	39.093	3.830	1.00 36.20
ATOM	1167	CB	ALA	155	46.522	38.771	2.621	1.00 36.22
ATOM	1168	c	ALA	155	44.412	39.864	3.387	1.00 36.20
ATOM	1169	ō	ALA	155	43.490	39.289	2.820	1.00 36.87
ATOM	1170	N	GLY	156	44.402	41.168	3.642	1.00 36.26
ATOM	1171	CA	GLY	156	43.279	41.997	3.245	1.00 37.08
ATOM	1172	c	GLY	156	43.481	43.446	3.647	1.00 38.10
ATOM	1173	ō	GLY	156	44.027	43.727	4.711	1.00 38.52
ATOM	1174	N	ILE	157	43.052	44.377	2.805	1.00 39.16
ATOM	1175	CA	ILE	157	43.203	45.789	3.125	1.00 41.42

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MOTA	1176	СВ	ILE	157	43.389	46.646	1.842	1.00 42.84
MOTA	1177	CG2	ILE	157	44.844	46.550	1.342	1.00 44.32
ATOM	1178	CG1	ILE	157	42.399	46.193	0.761	1.00 43.93
ATOM	1179	CD1	ILE	157	42.630			1.00 44.55
ATOM	1180	CDI	ILE	157	42.010	46.838	-0.615	1.00 42.26
						46.331	3.921	
ATOM	1181	0	ILE	157	40.864	45.912	3.732	1.00 42.28
MOTA	1182	N	LEU	158	42.300	47.259	4.824	1.00 42.54
MOTA	1183	CA	LEU	158	41.283	47.873	5.648	1.00 43.22
MOTA	1184	CB	LEU	158	41.928	48.504	6.884	1.00 44.12
MOTA	1185	CG	LEU	158	41.090	49.514	7.670	1.00 44.84
MOTA	118-6		LEU	158	40.020	48.782	8.472	1.00 45.23
MOTA	1187		LEU	158	42.006	50.320	8.590	1.00 45.09
ATOM	1188	C	LEU	158	40.548	48.947	4.855	1.00 43.56
ATOM	1189	0	LEU	158	40.984	50.099	4.801	1.00 43.77
ATOM	1190	N	LEU	159	39.434	48.569	4.239	1.00 43.40
ATOM	1191	CA	LEU	159	38.634	49.508	3.465	1.00 43.01
MOTA	1192	CB	LEU	159	37.238	48.935	3.280	1.00 43.36
MOTA	1193	CG	LEU	159	37.279	47.599	2.539	1.00 43.44
MOTA	1194	CD1	LEU	159	36.020	46.808	2.829	1.00 44.00
MOTA	1195	CD2	LEU	159	37.443	47.857	1.050	1.00 42.93
MOTA	1196	С	LEU	159	38.564	50.879	4.139	1.00 42.62
MOTA	1197	0	LEU	159	38.745	51.905	3.488	1.00 43.03
MOTA	1198	N	ASN	160	38.297	50.902	5.440	1.00 42.20
MOTA	1199	CA	ASN	160	38.243	52.169	6.170	1.00 41.99
MOTA	1200	CB	ASN	160	37.347	. 53.197	5.447	1.00 42.23
MOTA	1201	CG	ASN	160	35.913	52.733	5.295	1.00 43.38
MOTA	1202	OD1	ASN	160	35.225	53.102	4.334	1.00 42.38
ATOM	1203	ND2	ASN	160	35.444	51.934	6.250	1.00 44.48
MOTA	1204	С	ASN	160	37.813	51.988	7.616	1.00 41.13
MOTA	1205	0	ASN	160	37.359	50.913	8.011	1.00 41.17
ATOM	1206	N	TRP	161	37.980	53.043	8.403	1.00 40.24
ATOM	1207	CA	TRP	161	37.652	53.004	9.824	1.00 39.69
MOTA	1208	СВ	TRP	161	38.522	54.003	10.602	1.00 39.33
ATOM	1209	CG	TRP	161	39.987	53.640	10.769	1.00 39.07
ATOM	1210	CD2		161	40.527	52.469	11.411	1.00 38.63
ATOM	1211	CE2		161	41.931	52.616	11.438	1.00 38.27
ATOM	1212	CE3	TRP	161	39.960	51.317	11.972	1.00 38.43
ATOM	1213	CD1	TRP	161	41.060	54.417	10.436	1.00 38.40
ATOM	1214	NE1	TRP	161	42.228	53.812	10.840	1.00 38.42
MOTA	1215	CZ2		161	42.778	51.659	12.000	1.00 38.26
ATOM	1216	CZ3	TRP	161	40.809	50.357	12.538	1.00 38.07
ATOM	1217	CH2	TRP	161	42.200	50.540	12.545	1.00 38.37
ATOM	1218	С	TRP	161	36.196	53.301	10.150	1.00 39.07
MOTA	1219	0	TRP	161	35.578	54.193	9.562	1.00 39.38
ATOM	1220	N	THR	162	35.668	52.555	11.114	1.00 38.45
ATOM	1221	CA	THR	162	34.302	52.734	11.593	1.00 38.37
ATOM	1222	CB	THR	162	33.381	51.600	11.125	1.00 37.71
ATOM	1223	OG1		162	33.926	50.338	11.548	1.00 37.02
ATOM	1224	CG2		162	33.226	51.635	9.617	1.00 36.52
ATOM	1225	c	THR	162	34.357	52.702	13.121	1.00 38.24
ATOM .		0	THR	162	35.405	52.443	13.703	1.00 37.86
ATOM	1227	N	LYS	163	33.231	52.968	13.770	1.00 38.99
ATOM	1228	CA	LYS	163	33.192	52.941	15.222	1.00 39.72
ATOM	1229	СВ	LYS	163	33.510	51.528	15.728	1.00 38.16
ATOM	1230	CG	LYS	163	32.467	50.487	15.311	1.00 36.62
ATOM	1231	CD	LYS	163	32.727	49.108	15.918	1.00 34.66
ATOM	1232	CE	LYS	163	33.829	48.349	15.195	1.00 33.22
ATOM	1233	NZ	LYS	163	34.068	47.031	15.850	1.00 32.19
ATOM	1234	C	LYS	163	34.142	53.956	15.848	1.00 40.71
	2237	-	210	203	34.142	33.930	13.040	1.00 10.74

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ATOM	1235	0	T W.C	1.62	74 600	E2 =02	1.6.004	1 00 10 60
ATOM	1235	N	LYS	163 164	34.690	53.723	16.931	1.00 40.69 1.00 41.81
ATOM	1237	CA	GLY	164	34.338 35.187	55.076	15.156	1.00 41.01
ATOM						56.139	15.672	
ATOM	1238 1239	C	GLY	164 164	36.685	56.031	15.463	1.00 45.41
			GLY		37.375	57.055	15.381	1.00 45.25
MOTA	1240	N	PHE	165	37.190	54.802	15.397	1.00 47.06
MOTA	1241	CA	PHE	165	38.613	54.560	15.197	1.00 48.70
MOTA	1242	CB	PHE	165	38.852	53.117	14.767	1.00 47.20
MOTA	1243	CG	PHE	165	39.290	52.222	15.870	1.00 45.64
ATOM	1244	CD1		165	38.443	51.937	16.929	1.00 45.87
ATOM	1245	CD2	PHE	165	40.544	51.632	15.833	1.00 45.19
ATOM	1246	CE1		165	38.840	51.064	17.945	1.00 46.28
MOTA	1247	CE2		165	40.952	50.763	16.834	1.00 45.80
MOTA	1248	CZ	PHE	165	40.098	50.475	17.896	1.00 45.96
ATOM	1249	C	PHE	165	39.250	55.471	14.154	1.00 50.94
ATOM	1250	0	PHE	165	38.633	55.823	13.143	1.00 50.36
ATOM	1251	N	LYS	166	40.500	55.838	14.415	1.00 53.77
ATCM	1252	CA	LYS	166	41.275	56.680	13.514	1.00 56.56
ATOM	1253	CB	LYS	166	41.050	58.170	13.822	1.00 56.16
ATOM	1254	CG	LYS	166	39.720	58.697	13.290	1.00 56.44
MOTA	1255	CD	LYS	166	39.524	58.320	11.812	1.00 56.54
MOTA	1256	CE	LYS	166	38.131	58.694	11.305	1.00 56.74
MOTA	1257	NZ	LYS	166	37.863	58.198	9.922	1.00 56.86
MOTA	1258	С	LYS	166	42.751	56.322	13.640	1.00 58.33
MOTA	1259	0	LYS	166	43.180	55.747	14.651	1.00 58.69
MOTA	1260	N	ALA	167	43.510	56.647	12.597	1.00 59.76
MOTA	1261	CA	ALA	167	44.943	56.375	12.543	1.00 61.43
MOTA	1262	CB	ALA	167	45.220	54.901	12.834	1.00 60.92
ATOM	1263	C	ALA	167	45.401	56.725	11.137	1.00 62.76
ATOM	1264	0		. 167	45.147	55.967	10.197	1.00 63.38
MOTA	1265	N	SER	168	46.066	57.872	10.999	1.00 63.98
MOTA	1266	CA	SER	168	46.556	58.345	9.704	1.00 64.43
MOTA	1267	CB	SER	168	47.636	59.414	9.903	1.00 64.96
MOTA	1268	OG	SER	168	47.130	60.546	10.594	1.00 65.76
ATOM	1269	С	SER	168	47.115	57.216	8.846	1.00 64.59
ATOM	1270	0	SER	168	47.805	56.322	9.347	1.00 64.35
ATOM	1271	N	GLY	169	46.800	57.260	7.553	1.00 64.75
ATOM	1272	CA	GLY	169	47.280	56.245	6.632	1.00 65.55
ATOM ATOM	1273 1274	C	GLY	169 169	47.158	54.821	7.142	1.00 65.88
ATOM	1275	N	GLY	170	48.151	54.097	7.255	1.00 65.72
ATOM	1275	CA	ALA	170	45.936 45.699	54.416 53.065	7.465	1.00 66.32 1.00 66.82
ATOM	1277	CB	ALA	170	44.930	53.100	7.947 9.256	1.00 66.65
ATOM	1278	C	ALA	170	44.890			
ATOM	1279	ō	ALA	170	45.209	52.346 51.226	6.879	1.00 67.02 1.00 67.31
ATOM	1280	N	GLU	171	43.209	53.017	6.477	1.00 66.85
ATOM	1281	CA	GLU	171	42.979	52.463	5.387	1.00 66.80
MOTA	1282	СВ	GLU	171	41.705	53.292	5.287	1.00 65.80
ATOM	1283	CG	GLU	171	41.958	54.783	5.279	1.00 69.27
MOTA	1284	CD	GLU	171	40.850	55.552	4.590	1.00 69.27
ATOM	1285	OE1		171	40.789	55.506	3.340	1.00 70.17
ATOM	1286	OE2		171	40.789	56.191	5.296	1.00 70.43
ATOM	1287	C	GLU	171	43.666	52.427	4.032	1.00 65.92
ATOM	1288	0	GLU	171	44.469	53.301	3.711	1.00 66.22
ATOM	1289	N	GLY	172	43.339	51.408	3.242	1.00 64.69
ATOM	1290	CA	GLY	172	43.333	51.265	1.925	1.00 62.79
ATOM	1291	CA	GLY	172	45.096	50.312	1.882	1.00 62.79
ATOM	1292	0	GLY	172	45.493	49.884	0.805	1.00 61.61
ATOM	1292	N	ASN	173		49.884	3.045	1.00 61.39
ALOR	1233	14	MOIN	1/3	45.643	47.705	3.045	1.00 00.73

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ATOM	1294	CA	ASN	173	46.800	40 000		1 00 60 10
ATOM	1295					49.065	3.115	1.00 60.42
		CB	ASN	173	47.922	49.722	3.913	1.00 61.72
MOTA	1296	CG	ASN	173	48.035	51.201	3.631	1.00 62.78
ATOM	1297		ASN	173	48.367	51.605	2.515	1.00 63.29
MOTA	1298		ASN	173	47.741	52.024	4.637	1.00 63.06
ATOM	1299	С	ASN	173	46.463	47.747	3.771	1.00 59.26
MOTA	1300	0	ASN	173	45.440	47.624	4.430	1.00 59.57
ATOM	1301	N	ASN	174	47.336	46.763	3.598	1.00 58.79
MOTA	1302	CA	ASN	174	47.126	45.447	4.196	1.00 58.46
MOTA	1303	CB	ASN	174	48.264	44.495	3.793	1.00 57.45
ATOM	1304	CG	ASN	174	48.104	43.093	4.375	1.00 57.22
MOTA	1305	OD1	ASN	174	48.757	42.144	3.924	1.00 56.21
ATOM	1306	ND2	ASN	174	47.245	42.957	5.382	1.00 56.76
ATOM	1307	С	ASN	174	47.083	45.615	5.712	1.00 58.42
ATOM	1308	0	ASN	174	47.927	46.302	6.281	1.00 59.03
ATOM	1309	N	VAL	175	46.091	45.008	6.359	1.00 58.23
ATOM	1310	CA	VAL	175	45.966	45.106	7.809	1.00 57.79
ATOM	1311	CB	VAL	175	44.544	44.765	8.295	1.00 57.69
ATOM	1312	CG1	VAL	175	44.461	44.933	9.807	1.00 56.81
ATOM	1313	CG2	VAL	175	43.531	45.665	7.603	1.00 57.69
ATOM	1314	С	VAL	175	46.944	44.150	8.470	1.00 57.62
MOTA	1315	0	VAL	175	47.734	44.560	9.319	1.00 57.89
ATOM	1316	N	VAL	176	46.896	42.878	8.086	1.00 57.24
ATOM	1317	CA	VAL	176	47.818	41.904	8.660	1.00 57.25
ATOM	1318	CB	VAL	176	47.638	40.501	8.037	1.00 57.27
ATOM	1319		VAL	176	48.597	39.511	8.701	1.00 56.21
ATOM	1320	CG2		176	46.196	40.035	8.199	1.00 56.28
ATOM	1321	C	VAL	176	49.232	42.396	8.362	1.00 57.38
ATOM	1322	ō	VAL	176	50.212	41.911	8.926	1.00 57.30
ATOM	1323	N	GLY	177	49.319	43.374	7.467	1.00 57.41
ATOM	1324	CA	GLY	177	50.605	43.939	7.103	1.00 57.60
ATOM	1325	c	GLY	177	51.135	44.878	8.170	1.00 57.50
ATOM	1326	ō	GLY	177	52.171	44.605	8.781	1.00 58.09
ATOM	1327	N	LEU	178	50.425	45.982	8.396	1.00 56.68
ATOM	1328	CA	LEU	178	50.837	46.959	9.396	1.00 55.42
ATOM	1329	CB	LEU	178	49.710	47.968	9.646	1.00 55.02
ATOM	1330	CG	LEU	178	49.394	48.906	8.466	1.00 54.15
ATOM	1331		LEU	178	48.158	49.743	8.766	1.00 53.80
ATOM	1332		LEU	178	50.588	49.815	8.197	1.00 54.17
ATOM	1333	c	LEU	178	51.247	46.279	10.701	1.00 54.84
ATOM	1334	ō	LEU	178	52.177	46.717	11.375	1.00 55.07
ATOM	1335	N	LEU	179	50.575	45.192	11.050	1.00 53.85
ATOM	1336	CA	LEU	179	50.917	44.491	12.274	1.00 53.55
ATOM	1337	CB	LEU	179	49.882	43.409	12.582	1.00 52.75
ATOM	1338	CG	LEU	179	50.099	42.671	13.907	1.00 52.73
ATOM	1339	CD1		179	49.689	43.580	15.056	1.00 51.63
ATOM	1340	CD2		179	49.286	41.381	13.935	1.00 51.34
ATOM	1341	c	LEU	179	52.286	43.845	12.128	1.00 54.26
ATOM	1342	Ö	LEU	179	53.070	43.796	13.075	1.00 54.60
ATOM	1342	N	ARG	180	52.576	43.796	10.932	1.00 54.59
ATOM	1344	CA	ARG	180	52.576			1.00 54.59
ATOM	1345	CB	ARG	180	53.824	42.679 41.911	10.688	1.00 52.59
ATOM	1345	CG	ARG	180	53.824	40.498	9.357	1.00 50.37
ATOM	1345	CD	ARG	180			9.515	
ATOM		NE		180	53.276	39.702	8.223	1.00 47.24
	1348	CZ	ARG		52.610	38.420	8.425	1.00 45.06
MOTA	1349		ARG	180	51.979	37.754	7.462	1.00 43.97
MOTA	1350	NH1		180	51.935	38.256	6.226	1.00 42.53
MOTA	1351		ARG	180	51.366	36.601	7.735	1.00 42.95
ATOM	1352	С	ARG	180	55.059	43.605	10.732	1.00 54.76

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ATOM	1353	0	ARG	180	56.009	42 242		1.00 54.65
ATOM	1354	N	ASP	181		43.343	11.473	
ATOM	1355			181	55.036	44.681	9.951	1.00 55.34
		CA	ASP		56.169	45.593	9.972	1.00 56.60
ATOM	1356	CB	ASP	181	56.266	46.386	8.649	1.00 56.43
ATOM	1357	CG	ASP	181	55.132	47.382	8.448	1.00 55.64
MOTA	1358		ASP	181	54.658	47.483	7.294	1.00 55.20
MOTA	1359		ASP	181	54.734	48.076	9.416	1.00 55.23
MOTA	1360	C	ASP	181	56.115	46.514	11.199	1.00 57.64
MOTA	1361	0	ASP	181	56.510	47.635	11.153	1.00 57.96
MOTA	1362	N	ALA	182	55.634	45.947	12.303	1.00 57.87
MOTA	1363	CA	ALA	182	55.524	46.646	13.577	1.00 57.84
ATOM	1364	CB	ALA	182	54.078	47.048	13.836	1.00 58.19
ATOM	1365	C	ALA	182	56.013	45.683	14.657	1.00 57.83
ATOM	1366	0	ALA	182	56.681	46.094	15.611	1.00 58.32
ATOM	1367	N	ILE	183	55.669	44.404	14.505	1.00 57.35
ATCM	1368	CA	ILE	183	56.109	43.381	15.448	1.00 57.40
MOTA	1369	CB	ILE	183	55.374	42.036	15.233	1.00 56.09
MOTA	1370	CG2	ILE	183	56.025	40.932	16.074	1.00 55.25
ATOM	1371	CG1	ILE	183	53.904	42.174	15.628	1.00 55.30
MOTA	1372	CD1	ILE	183	53.115	40.831	15.505	1.00 54.14
ATOM	1373	c	ILE	183	57.600	43.164	15.199	1.00 58.51
ATOM	1374	ō	ILE	183	58.294	42.531	16.002	1.00 59.24
ATOM	1375	N	LYS	184	58.093	43.689	14.077	1.00 59.04
ATOM	1376	CA	LYS	184	59.508	43.550	13.757	1.00 59.19
ATOM	1377	CB	LYS	184	59.719			1.00 59.15
ATOM	1378	CG	LYS	184	59.356	43.243	12.268	1.00 58.36
ATOM	1379	CD	LYS	184	59.566			
ATOM	1380	CE	LYS	184		43.897	9.868	1.00 58.59
ATOM	1381	NZ	LYS	184	58.637	42.735	9.500	1.00 59.26
ATOM					58.751	42.306	8.067	1.00 59.63
	1382	C	LYS	184	60.270	44.806	14.155	1.00 59.27
MOTA	1383		LYS	184	61.382	44.705	14.667	1.00 59.28
ATOM	1384	N	ARG	185	59.695	45.984	13.923	1.00 59.21
MOTA	1385	CA	ARG	185	60.383	47.211	14.331	1.00 59.69
MOTA	1386	CB	ARG	185	59.545	48.458	14.060	1.00 59.70
MOTA	1387	CG	ARG	185	59.278	48.772	12.610	1.00 60.85
MOTA	1388	CD	ARG	185	59.138	50.280	12.443	1.00 60.89
MOTA	1389	NE	ARG	185	58.121	50.628	11.459	1.00 62.26
ATOM	1390	CZ	ARG	185	56.819	50.403	11.620	1.00 61.84
MOTA	1391		ARG	185	56.372	49.828	12.731	1.00 61.22
ATOM	1392	NH2		185	55.966	50.754	10.666	1.00 62.23
ATOM	1393	C	ARG	185	60.574	47.104	15.836	1.00 60.41
ATOM	1394	0	ARG	185	61.630	47.430	16.384	1.00 60.45
ATOM	1395	N	ARG	186	59.518	46.633	16.489	1.00 61.07
ATOM	1396	CA	ARG	186	59.489	46.460	17.933	1.00 61.42
ATOM	1397	CB	ARG	186	58.066	46.055	18.358	1.00 61.16
ATOM	1398	CG	ARG	186	57.666	46.433	19.786	1.00 61.08
ATOM	1399	CD	ARG	186	58.249	45.473	20.828	1.00 60.87
ATOM	1400	NE	ARG	186	57.917	45.894	22.188	1.00 61.44
ATOM	1401	CZ	ARG	186	58.294	45.246	23.288	1.00 60.67
ATOM	1402	NH1	ARG	186	59.024	44.133	23.201	1.00 60.28
ATOM	1403	NH2	ARG	186	57.942	45.712	24.481	1.00 61.46
ATOM	1404	C	ARG	186	60.516	45.399	18.344	1.00 61.85
ATOM	1405	0	ARG	186	60.980	44.610	17.514	1.00 62.16
ATOM	1406	N	GLY	187	60.873	45.401	19.628	1.00 62.07
MOTA	1407	CA	GLY	187	61.843	44.455	20.157	1.00 62.22
MOTA	1408	C	GLY	187	61.591	43.017	19.754	1.00 62.50
MOTA	1409	ō	GLY	187	60.541	42.692	19.202	1.00 62.37
ATOM	1410	N	ASP	188	62.556	42.148	20.036	1.00 63.08
ATOM	1411	CA	ASP	188	62.414	40.746	19.684	1.00 62.67
2021	T-4-T	0.1	*****	100	02.414	40.740	17.004	1.00 02.07

Figur 4

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ATOM	1412	СВ	ASP	188	63.465	39.873	20.373	1.00 61.80
ATOM	1413	CG	ASP	188	63.403			1.00 60.64
ATOM	1414		ASP	188		38.409	20.468	
		OD1			62.125	38.107	21.289	1.00 60.77
ATOM	1415	OD2	ASP	188	63.565	37.563	19.715	1.00 60.43
ATOM	1416	C	ASP	188	61.047	40.193	20.022	1.00 63.58
ATOM	1417	0	ASP	188	60.441	40.539	21.044	1.00 62.69
MOTA	1418	N	PHE	189	60.599	39.309	19.138	1.00 64.49
MOTA	1419	CA	PHE	189	59.327	38.632	19.249	1.00 64.75
MOTA	1420	CB	PHE	189	58.233	39.629	19.598	1.00 64.84
MOTA	1421	CG	PHE	189	56.886	39.010	19.689	1.00 65.46
ATOM	1422	CD1	PHE	189	56.707	37.824	20.402	1.00 65.54
ATOM	1423	CD2	PHE	189	55.795	39.592	19.052	1.00 65.28
ATOM	1424	CE1	PHE	189	55.455	37.224	20.481	1.00 65.61
MOTA	1425	CE2	PHE	189	54.542	39.007	19.122	1.00 65.71
MOTA	1426	CZ	PHE	189	54.369	37.819	19.839	1.00 65.57
ATOM	1427	С	PHE	189	59.018	37.952	17.919	1.00 65.33
MOTA	1428	0	PHE	189	58.921	38.609	16.881	1.00 64.91
ATOM	1429	N	GLU	190	58.879	36.631	17.956	1.00 66.13
ATOM	1430	CA	GLU	190	58.584	35.854	16.752	1.00 66.57
ATOM	1431	CB	GLU	190	59.387	34.545	16.755	1.00 66.34
ATOM	1432	CG	GLU	190	60.778	34.649	17.389	1.00 64.66
ATOM	1433	CD	GLU	190	61.908	34.356	16.411	1.00 64.02
ATOM	1434	OE1	GLU	190	63.054	34.161	16.874	1.00 63.09
ATOM	1435	OE2	GLU	190	61.658	34.327	15.186	1.00 63.04
ATOM	1436	С	GLU	190	57.093	35.528	16.745	1.00 67.09
ATOM	1437	0	GLU	190	56.609	34.828	17.638	1.00 67.36
ATOM	1438	N	MSE	191	56.367	36.030	15.747	1.00 67.05
ATOM	1439	CA	MSE	191	54.928	35.775	15.666	1.00 66.65
ATOM	1440	СЗ	MSE	191	54.164	36.920	16.347	1.00 69.47
ATOM	1441	CG	MSE	191	52.867	36.492	17.037	1.00 72.30
ATOM	1442	SE	MSE	191	53.120	35.293	18.409	1.00 78.56
ATOM	1443	CE	MSE	191	51.941	35.893	19.581	1.00 75.88
MOTA	1444	Ċ	MSE	191	54.412	35.590	14.230	1.00 64.85
ATOM	1445	ō	MSE	191	54.399	36.538	13.435	1.00 64.30
MOTA	1446	N	ASP	192	53.977	34.368	13.910	1.00 62.82
MOTA	1447	CA	ASP	192	53.449	34.051	12.580	1.00 60.76
ATOM	1448	CB	ASP	192	53.774	32.607	12.207	1.00 61.24
ATOM	1449	CG	ASP	192	55.210	32.427	11.792	1.00 61.76
ATOM	1450	OD1		192	55.684	33.219	10.947	1.00 62.45
ATOM	1451	OD2		192	55.863	31.492	12.299	1.00 62.32
ATOM	1452	C	ASP	192	51.942	34.266	12.459	1.00 59.03
ATOM	1453	ō	ASP	192	51.143	33.375	12.767	1.00 58.37
ATOM	1454	N	VAL	193	51.567	35.453	11.991	1.00 57.00
ATOM	1455	CA	VAL	193	50.167	35.818	11.818	1.00 54.85
ATOM	1456	СВ	VAL	193	50.034	37.305	11.454	1.00 55.09
ATOM	1457		VAL	193	48.568	37.712	11.448	1.00 54.84
ATOM	1458	CG2	VAL	193	50.826	38.146	12.441	1.00 54.87
ATOM	1459	C	VAL	193	49.473	34.977	10.746	1.00 53.19
ATOM	1450	ō	VAL	193	49.500	35.303	9.555	1.00 52.03
ATOM	1461	N	VAL	194	48.854	33.894	11.205	1.00 51.82
ATOM	1462	CA	VAL	194	48.126	32.949	10.367	1.00 50.66
MOTA	1463	CB	VAL	194	47.841	31.644	11.174	1.00 51.08
ATOM	1464	CG1		194	46.686	30.860	10.554	1.00 52.09
ATOM	1465	CG2		194	49.091	30.778	11.211	1.00 52.09
ATOM	1466	CG2	VAL	194	46.798			1.00 51.33
ATOM	1467	0	VAL	194	46.798	33.498	9.808 8.602	1.00 49.40
ATOM	1468	N	ALA	195	45.813		10.683	1.00 49.40
ATOM	1469	CA	ALA	195	44.499	33.723	10.683	1.00 48.93
ATOM	1470	CB	ALA	195	44.499			
ALON	14/0	CD	LLL	133	43.40/	33.123	10.572	1.00 47.58

Figur 4

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ATOM	1471	c	ALA	195	43 000	35 546	10 700	1 00 46 60
ATOM	1472	0	ALA	195	43.992 44.344	35.546 35.996	10.760	1.00 46.68
ATOM	1473	N	MSE	196			11.851	
ATOM	1474	CA	MSE	196	43.157	36.182	9.940	1.00 45.43
ATOM	1475	CB			42.521	37.459	10.279	1.00 44.60
			MSE	196	43.079	38.623	9.451	1.00 45.32
ATOM	1476	CG	MSE	196	42.329	39.925	9.716	1.00 47.29
ATOM	1477	SE	MSE	196	42.937	41.426	8.852	1.00 53.21
ATOM	1478	CE	MSE	196	44.264	41.920	9.982	1.00 51.44
ATOM	1479	C	MSE	196	41.019	37.333	10.002	1.00 43.09
MOTA		. 0	MSE	196	40.610	36.973	8.892	1.00 43.71
MOTA	1481	N	VAL	197	40.190	37.631	10.996	1.00 40.47
MOTA	1482	CA	VAL	197	38.751	37.514	10.799	1.00 37.00
ATOM	1483	CB	VAL	197	38.240	36.228	11.458	1.00 37.31
ATOM	1484	CG1		197	38.840	35.004	10.766	1.00 36.64
MOTA	1485	CG2	VAL	197	38.643	36.217	12.914	1.00 36.88
ATOM	1486	C	VAL	197	37.991	38.710	11.354	1.00 35.22
ATOM	1487	0	VAL	197	38.561	39.544	12.057	1.00 35.21
ATOM	1488	N	ASN	198	36.708	38.801	11.015	1.00 33.39
ATOM	1489	CA	ASN	198	35.830	39.883	11.491	1.00 30.23
ATOM	1490	CB	ASN	198	34.740	40.175	10.446	1.00 30.65
ATOM	1491	CG	ASN	198	33.801	41.309	10.852	1.00 31.35
ATOM	1492		ASN	198	32.907	41.128	11.686	1.00 32.70
ATCM	1493	ND2	ASN	198	33.997	42.486	10.251	1.00 30.53
ATOM	1494	С	ASN	198	35.217	39.356	12.780	1.00 28.41
ATOM	1495	0	ASN	198	35.052	38.143	12.937	1.00 26.14
ATOM	1496	N	ASP	199	34.892	40.252	13.711	1.00 27.77
ATOM	1497	CA	ASP	199	34.325	39.816	14.990	1.00 26.87
ATOM	1498	CB	ASP	199	34.156	41.007	15.945	1.00 26.75
ATOM	1499	CG	ASP	199	33.254	42.097	15.396	1.00 26.24
ATOM	1500		ASP	199	33.221	42.292	14.167	1.00 25.90
ATOM	1501	OD2	ASP	199	32.587	42.777	16.205	1.00 26.19
ATOM	1502	С	ASP	199	33.027	39.034	14.843	1.00 26.43
ATCM	1503	0	ASP	199	32.715	38.188	15.684	1.00 27.02
ATOM	1504	N	THR	200	32.291	39.292	13.763	1.00 25.45
ATOM	1505	CA	THR	200	31.050	38.585	13.510	1.00 25.65
ATOM	1506	CB	THR	200	30.261	39.193	12.339	1.00 25.75
ATOM	1507	OG1	THR	200	31.008	39.044	11.130	1.00 26.04
ATOM	1508	CG2		200	30.002	40.672	12.573	1.00 26.48
ATOM	1509	C	THR	200	31.383	37.155	13.143	1.00 26.96
ATOM ATOM	1510 1511	O N	THR	200	30.832	36.211	13.712	1.00.27.62
ATOM	1512	CA	VAL	201	32.295	36.990	12.189	1.00 28.07
ATOM	1512	CB	VAL	201	32.695	35.654	11.742	1.00 28.50
ATOM	1513	CG1	VAL	201	33.785	35.726	10.665	1.00 29.26
ATOM	1514	CG2		201	34.056	34.332	10123	1.00 31.22
ATOM	1516			201	33.370	36.684	9.546	1.00 27.90
ATOM	1517	C	VAL	201	33.231	34.818	12.901	1.00 29.16
ATOM	1518	O N	ALA	201 202	32.816	33.676	13.101	1.00 29.44
ATOM	1519	CA	ALA	202	34.156	35.395	13.663	1.00 30.31
ATOM	1520	CB			34.752	34.710	14.812	1.00 32.23
ATOM ATOM	1521	CB	ALA	202 202	35.591	35.705	15.643	1.00 31.72
ATOM	1522	0	ALA	202	33.688	34.070	15.696	1.00 33.37
ATOM	1522	N	THR	202		32.894	16.073	1.00 34.14
ATOM	1524	CA	THR		32.667	34.858	16.019	1.00 34.41
ATOM	1525	CB	THR	203	31.566	34.422	16.870	1.00 35.37
ATOM	1525	OG1		203 203	30.614	35.604	17.117	1.00 36.27
					31.370	36.708	17.645	1.00 37.04
ATOM ATOM	1527 1528	CG2 C	THR	203 203	29.500	35.213	18.090	1.00 35.19
ATOM	1528	0			30.800	33.260	16.242	
ATOM	1329	U	THR	203	30.538	32.241	16.891	1.00 35.34

Figur 4

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MOTA	1530	N	MSE	204	30.433	33.415	14.978	1.00 36.89
ATOM	1531	CA	MSE	204	29.722	32.348	14.299	1.00 37.94
MOTA	1532	CB	MSE	204	29.582			1.00 37.34
ATOM	1533	CG	MSE	204		32.665	12.811	
	1534	SE			29.065	31.504	11.954	1.00 40.74
ATOM			MSE	204	29.135	31.967	10.181	1.00 45.75
MOTA	1535	CE	MSE	204	30.643	31.057	9.627	1.00 45.26
MOTA	1536	С	MSE	204	30.531	31.075	14.465	1.00 38.36
ATOM	1537	0	MSE	204	30.024	30.064	14.954	1.00 37.86
MOTA	1538	N	ILE	205	31.798	31.148	14.061	1.00 38.79
MOTA	1539	CA	ILE	205	32.696	30.008	14.137	1.00 40.09
MOTA	1540	CB	ILE	205	34.178	30.451	13.981	1.00 39.81
MOTA	1541	CG2	ILE	205	35.098	29.240	14.072	1.00 39.47
MOTA	1542	CG1		205	34.398	31.112	12.616	1.00 39.46
MOTA	1543	CD1	ILE	205	34.250	30.158	11.425	1.00 39.34
ATOM	1544	C	ILE	205	32.527	29.215	15.440	1.00 41.34
ATOM	1545	0	ILE	205	32.121	28.050	15.408	1.00 41.41
MOTA	1546	N	SER	206	32.812	29.830	16.584	1.00 42.01
ATOM	1547	CA	SER	206	32.683	29.112	17.849	1.00 43.71
MOTA	1548	CB	SER	206	32.999	30.038	19.013	1.00 43.57
MOTA	1549	OG	SER	206	32.149	31.163	18.971	1.00 44.54
ATOM	1550	C	SER	206	31.306	28.494	18.056	1.00 44.83
MOTA	1551	ō	SER	206	31.185	27.304	18.364	1.00 45.40
ATOM	1552	N	CYS	207	30.260	29.291	17.894	1.00 45.32
ATOM	1553	CA	CYS	207	28.912	28.764	18.079	1.00 48.14
ATOM	1554	CB	CYS	207	27.869	29.842	17.780	1.00 45.74
ATOM	1555	SG	CYS	207	27.946	31.264	18.883	1.00 42.50
ATOM	1556	c	CYS	207	28.666	27.551	17.186	1.00 50.79
ATOM	1557	ō	CYS	207	27.715	26.799	17.100	1.00 50.79
ATOM	1558	N	TYR	208	29.533	27.361	16.190	1.00 53.91
ATOM	1559	CA	TYR	208	29.418	26.243	15.247	1.00 56.61
ATOM	1560	CB	TYR	208	30.350	26.458	14.045	1.00 56.96
ATOM	1561	CG	TYR	208	30.370	25.303	13.062	1.00 57.29
ATOM	1562	CD1		208	29.307	25.090	12.182	1.00 57.29
ATOM	1563	CE1	TYR	208	29.307			1.00 57.54
ATOM	1564	CD2		208	31.448	24.025	11.280	1.00 57.54
ATOM	1565	CE2		208			13.019	
ATOM	1566	CZ	TYR	208	31.468	23.350	12.125	1.00 57.60
ATOM	1567	OH	TYR	208	30.404	23.163	11.258	1.00 57.47
ATOM	1568	C	TYR	208	30.435	22.126	10.360	1.00 57.71
MOTA	1569	0	TYR	208	29.705	24.867	15.854	1.00 58.12
ATOM	1570	N	TYR	209	28.874	23.960	15.773	1.00 58.61
ATOM	1571	CA	TYR	209	30.876	24.699	16.459	1.00 59.77
ATOM	1572	CB	TYR	209	31.198	23.399	17.028	1.00 61.36
ATOM	1573	CG		209	32.619	23.394	17.581	1.00 63.23
ATOM			TYR		33.648	23.401	16.472	1.00 65.26
	1574	CD1		209	34.058	24.595	15.876	1.00 66.13
ATOM	1575	CE1		209	34.959	24-594	14.807	1.00 67.31
ATOM	1576	CD2		209	34.165	22.206	15.973	1.00 65.88
ATOM	1577	CE2		209	35.062	22.193	14.906	1.00 66.79
MOTA	1578	CZ	TYR	209	35.457	23.386	14.328	1.00 67.37
MOTA	1579	OH	TYR	209	36.350	23.370	13.277	1.00 67.62
MOTA	1580	C	TYR	209	30.206	22.965	18.083	1.00 61.32
ATOM	1581	0	TYR	209	30.048	21.771	18.336	1.00 61.19
ATOM	1582	N	GLU	210	29.523	23.938	18.680	1.00 61.63
ATOM	1583	CA	GLU	210	28.524	23.658	19.701	1.00 61.05
MOTA	1584	CB	GLU	210	28.444	24.808	20.706	1.00 62.29
ATOM	1585	CG	GLU	210	27.539	24.499	21.884	1.00 65.45
ATOM	1586	CD	GLU	210	27.716	25.463	23.050	1.00 67.38
ATOM	1587		GLU	210	28.865	25.609	23.535	1.00 68.93
ATOM	1588	OE2	GLU	210	26.707	26.065	23.488	1.00 67.92

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Figur 4

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MOTA	1589	С	GLU	210	27.175	23.459	19.026	1.00 60.04
ATOM	1590	0	GLU	210	26.255	22.901	19.618	1.00 59.93
ATOM	1591	N	ASP	211				1.00 58.82
					27.073	23.920	17.780	
ATOM	1592	CA	ASP	211	25.849	23.797	16.984	1.00 57.80
ATOM	1593	CB	ASP	211	24.804	24.824	17.441	1.00 58.16
MOTA	1594	CG	ASP	211	23.504	24.730	16.653	1.00 58.25
MOTA	1595	OD1	ASP	211	22.490	25.299	17.111	1.00 57.88
MOTA	1596	OD2		211	23.495	24.096	15.572	1.00 58.65
MOTA	1597	C	ASP	211	26.173	23.993	15.503	1.00 56.54
MOTA	1598	0	ASP	211	26.351	25.116	15.037	1.00 56.17
MOTA	1599	N	HIS	212	26.234	22.884	14.773	1.00 55.81
ATOM	1600	CA	HIS	212	26.577	22.884	13.351	1.00 55.26
ATOM	1601	CB	HIS	212	26.699	21.442	12.852	1.00 57.87
ATOM	1602	CG	HIS	212	27.816	20.678	13.493	1.00 61.52
ATOM	1603		HIS	212	27.815	19.527	14.205	1.00 62.63
MOTA	1604		HIS	212	29.127	21.110	13.460	1.00 62.80
MOTA	1605		HIS	212	29.884	20.258	14.127	1.00 63.70
ATOM	1606		HIS	212	29.114	19.288	14.590	1.00 63.71
ATOM	1607	С	HIS	212	25.665	23.656	12.412	1.00 53.29
ATOM	1608	0	HIS	212	26.014	23.883	11.251	1.00 52.77
ATOM	1609	M	GLN	213	24.496	24.058	12.895	1.00 51.08
ATOM	1610	CA	GLN	213	23.579	24.790	12.037	1.00 48.22
ATOM	1611	CB	GLN	213	22.135	24.347	12.298	1.00 49.39
ATOM	1612	CG	GLN	213	21.957	22.839	12.130	1.00 50.76
MOTA	1613	CD	GLN	213	20.507	22.410	11.965	1.00 51.82
ATOM	1614	OE1	GLN	213	19.653	22.721	12.803	1.00 52.48
ATOM	1615	NE2	GLN	213	20.223	21.679	10.883	1.00 51.72
ATOM	1616	С	GLN	213	23.746	26.289	12.202	1.00 45.19
ATOM	1617	0	GLN	213	22.978	27.077	11.654	1.00 45.00
MOTA	1618	N	CYS	214	24.759	26.686	12.957	1.00 41.87
MOTA	1619	CA	CYS	214	25.015	28.105	13.122	1.00 39.08
MOTA	1620	CB	CYS	214	25.907	28.386	14.332	1.00 39.18
MOTA	1621	SG	CYS	214	26.281	30.175	14.542	1.00 40.32
ATOM	1622	C	CYS	214	25.743	28.530	11.859	1.00 36.43
ATOM	1623	0	CYS	214	26.915	28.214	11.689	1.00 36.06
ATOM	1624	N	GLU	215	25.046	29.223	10.967	1.00 33.00
ATOM	1625	CA	GLU	215	25.664	29.672	9.736	1.00 30.60
ATOM	1626	CB	GLU	215	25.056	28.960	8.541	1.00 31.95
MOTA	1627	CG	GLU	215	25.289	27.466	8.561	1.00 33.57
MOTA	1628	CD	GLU	215	24.973	26.827	7.233	1.00 35.80
MOTA	1629	0E1		215	25.719	27.094	6.264	1.00 37.32
ATOM	1630	OE2		215	23.978	26.064	7.156	1.00 37.21
ATOM	1631	C	GLU	215	25.518	31.162	9.563	1.00 28.84
ATOM	1632	0	GLU	215	25.665	31.687	8.459	1.00 28.39
ATOM	1633	N	VAL	216	25.243	31.847	10.669	1.00 26.45
ATOM	1634	CA	VAL	216	25.083	33.291	10.648	1.00 23.67
MOTA	1635	CB	VAL	216	23.589	33.706	10.607	1.00 23.44
ATOM	1636		VAL	216	23.485	35.214	10.492	1.00 22.72
ATOM	1637	CG2	VAL	216	22.875	33.031	9.449	1.00 22.30
ATOM	1638	C	VAL	216	25.671	33.858	11.921	1.00 22.20
ATOM	1639	0	VAL	216	25.444	33.328	13.006	1.00 22.86
ATOM	1640	N	GLY	217	26.423	34.939	11.793	1.00 21.40
MOTA	1641	CA	GLY	217	26.997	35.554	12.965	1.00 21.14
ATOM	1642	C	GLY	217	26.524	36.994	13.022	1.00 22.30
MOTA	1643	0	GLY	217	26.432	37.677	11.983	1.00 22.05
ATOM	1644	N	MSE	218	26.201	37.454	14.228	1.00 23.03
ATOM	1645	CA	MSE	218	25.748	38.815	14.414	1.00 23.03
ATOM	1646	CB	MSE	218	24.208	38.880	14.445	1.00 25.98
ATOM	1647	CG	MSE	218	23.647	40.306	14.646	1.00 28.99

Figur 4

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MOTA	1640	C D	MCE	210	21 226			4 00 05 04
	1648	SE CE	MSE	218	21.806	40.486	14.543	1.00 35.34
MOTA	1649 1650	C	MSE	218	21.273	39.804	16.207	1.00 31.95
ATOM ATOM	1651	0	MSE	218 218	26.320	39.405	15.694	1.00 21.99
					26.425	38.738	16.724	1.00 22.34
MOTA	1652	N	ILE	219	26.694	40.670	15.606	1.00 21.28
ATOM	1653	CA	ILE	219	27.240	41.402	16.720	1.00 20.85
MOTA	1654	CB	ILE	219	28.702	41.840	16.449	1.00 20.74
ATOM	1655	CG2	ILE	219	29.164	42.757	17.558	1.00 19.65
ATOM	1656	CG1	ILE	219	29.623	40.627	16.335	1.00 19.32
ATOM	1657	CD1	ILE	219	29.656	39.770	17.596	1.00 20.63
MOTA	1658	С	ILE	219	26.413	42.676	16.838	1.00 21.47
ATOM	1659	0	ILE	219	26.297	43.431	15.868	1.00 21.30
ATOM	1660	N	VAL	220	25.823	42.908	18.003	1.00 21.91
ATOM	1661	CA	VAL	220	25.059	44.135	18.224	1.00 22.49
ATOM	1662	CB	VAL	220	23.563	43.873	18.479	1.00 22.04
ATOM	1663		VAL	220	22.815	45.183	18.425	1.00 21.50
MOTA	1664		VAL	220	23.007	42.901	17.463	1.00 22.03
MOTA	1665	С	VAL	220	25.650	44.775	19.477	1.00 23.27
MOTA	1666	0	VAL	220	25.095	44.642	20.575	1.00 23.94
MOTA	1667	N	GLY	221	26.795	45.436	19.312	1.00 22.78
ATOM	1668	CA	GLY	221	27.448	46.063	20.443	1.00 22.86
MOTA	1669	С	GLY	221	27.728	47.509	20.138	1.00 23.75
MOTA	1670	0	GLY	221	26.816	48.264	19.828	1.00 25.09
MOTA	1671	N	THR	222	28.988	47.906	20.233	1.00 24.06
MOTA	1672	CA	THR	222	29.375	49.277	19.939	1.00 24.06
MOTA	1673	CB	THR	222	30.893	49.423	19.960	1.00 24.59
MOTA	1674	OG1	THR	222	31.377	49.051	21.258	1.00 25.00
MOTA	1675	CG2	THR	222	31.299	50.860	19.640	1.00 24.67
MOTA	1676	С	THR	222	28.888	49.530	18.533	1.00 24.09
MOTA	1677	0	THR	222	28.248	50.530	18.259	1.00 24.72
MOTA	1678	N	GLY	223	29.211	48.597	17.646	1.00 24.40
MOTA	1679	CA	GLY	223	28.790	48.686	16.262	1.00 24.65
ATOM	1680	С	GLY	223	27.797	47.560	16.020	1.00 25.05
ATOM	1681	0	GLY	223	27.478	46.779	16.936	1.00 25.80
ATOM	1682	N	CYS	224	27.298	47.453	14.798	1.00 24.73
ATOM	1683	CA	CYS	224	26.338	46.405	14.504	1.00 24.18
MOTA	1684	CB	CYS	224	24.928	46.958	14.682	1.00 24.47
MOTA	1685	SG	ĊYS	224	23.640	45.925	13.998	1.00 25.11
ATOM ATOM	1686 1687	C	CYS	224	26.550	45.895	13.085	1.00 23.65
ATOM	1688	N	CYS	224 225	26.618	46.683	12.144	1.00 24.07
ATOM	1689	CA	ASN	225	26.650 26.883	44.578	12.941	1.00 23.06
ATOM	1690	CB	ASN	225	28.346	43.963	11.638 11.210	1.00 23.27 1.00 26.15
ATOM	1691	CG	ASN	225	28.831	44.230	10.098	1.00 27.94
ATOM	1692		ASN	225	28.271			1.00 27.34
ATOM	1693		ASN	225	29.878	43.265	8.997 10.393	1.00 29.23
ATOM	1694	C	ASN	225	26.603	42.459	11.740	1.00 21.80
ATOM	1695	Ö	ASN	225	26.291	41.954	12.827	1.00 20.54
ATOM	1696	N	ALA	225	26.709	41.759	10.610	1.00 20.54
ATOM	1697	CA	ALA	226	26.478	40.322	10.566	1.00 19.47
ATOM	1698	CB	ALA	226	24.994	40.322	10.566	1.00 20.99
ATOM	1699	C	ALA	226	27.194	39.723	9.378	1.00 20.33
MOTA	1700	Ö	ALA	226	27.529	40.428	8.415	1.00 18.72
MOTA	1701	N	CYS	227	27.404	38.415	9.439	1.00 17.37
ATOM	1702	CA	CYS	227	28.077	37.675	8.368	1.00 19.35
ATOM	1703	CB	CYS	227	29.523	37.396	8.751	1.00 18.42
MOTA	1704	SG	CYS	227	29.556	36.326	10.207	1.00 20.13
ATOM	1705	C	CYS	227	27.331	36.352	8.291	1.00 19.81
ATOM	1706	ō	CYS	227	26.702	35.951	9.280	1.00 20.62
011	1100	9	015	221	20.702	33.331	5.200	1.00 20.02

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ATOM	1707	N	TYR	228	27.402	35.668	7.148	1.00 20.49
ATOM	1708	CA	TYR	228	26.705	34.384	6.989	1.00 20.56
ATOM	1709	СЗ	TYR	228	25.242	34.633	6.624	1.00 17.90
ATOM	1710	CG	TYR	228	25.096	35.134	5.204	1.00 15.65
ATOM	1711	CD1	TYR	228	24.922	34.249	4.145	1.00 15.81
MOTA	1712	CE1	TYR	228	24.885	34.701	2.823	1.00 15.89
ATOM	1713	CD2	TYR	228	25.221	36.483	4.913	1.00 15.28
ATOM	1714	CE2	TYR	228	25.186	36.949	3.601	1.00 16.08
MOTA	1715	CZ	TYR	228	25.022	36.051	2.564	1.00 16.76
MOTA	1716	OH	TYR	228	25.033	36.505	1.263	1.00 18.93
ATOM	1717	C	TYR	228	27.345	33.539	5.887	1.00 22.19
ATOM	1718	o	TYR	228	28.174	34.024	5.112	1.00 21.49
ATOM	1719	N	MSE	229	25.928	32.278	5.808	1.00 24.74
ATOM	1720	CA	MSE	229	27.438	31.349	4.808	1.00 26.69
ATOM	1721	CB	MSE	229	27.342	29.918	5.339	1.00 28.61
ATOM	1722	CG	MSE	229	28.167	29.637	6.598	1.00 32.37
ATOM	1723	SE	MSE	229	29.987	30.056	6.460	1.00 41.17
MOTA	1724	CE	MSE	229	30.544	28.874	5.098	1.00 36.30
MOTA	1725	c	MSE	229	26.663	31.470	3.481	1.00 27.83
ATOM	1726	ō	MSE	229	25.535	30.994	3.363	1.00 28.02
ATOM	1727	N	GLU	230	27.282	32.109	2.492	1.00 29.19
ATOM	1728	CA	GLU	230	26.688	32.296	1.172	1.00 29.81
MOTA	1729	CB	GLU	230	27.165	33.623	0.577	1.00 30.83
ATCM	1730	CG	GLU	230	26.685	33.922	-0.843	1.00 32.33
ATOM	1731	CD	GLU	230	25.173	33.825	-0.989	1.00 34.04
ATOM	1732	OE1	GLU	230	24.663	32.698	-1.222	1.00 34.43
ATOM	1733	OE2	GLU	230	24.497	34.878	-0.858	1.00 33.65
MOTA	1734	C	GLU	230	27.127	31.143	0.282	1.00 30.91
ATOM	1735	0	GLU	230	27.958	30.319	0.685	1.00 30.80
MOTA	1736	N	GLU	231	26.562	31.078	-0.923	1.00 32.47
ATCM	1737	CA	GLU	231	26.885	30.024	-1.883	1.00 34.04
MOTA	1738	CB	GLU	231	25.668	29.696	-2.745	1.00 34.21
MOTA	1739	CG	GLU	231	24.408	29.396	-1.979	1.00 34.89
MOTA	1740	CD	GLU	231	24.452	28.054	-1.296	1.00 36.36
MOTA	1741	OE1		231	24.745	27.064	-2.002	1.00 36.80
ATOM	1742	OE2		231	24.182	27.981	-0.067	1.00 36.72
MOTA	1743	C	GLU	231	27.997	30.550	-2.777	1.00 35.65
ATOM	1744	0	ĠĽU	231	27.889	31.663	-3.304	1.00 35.42
MOTA	1745	N	MSE	232	29.060	29.758	-2.952	1.00 37.13
MOTA	1746	CA	MSE	232	30.188	30.181	-3.780	1.00 38.19
MOTA	1747	CB	MSE	232	31.191	29.036	-3.935	1.00 41.27
ATOM	1748	CG	MSE	232	32.195	28.912	-2.765	1.00 45.40
MOTA MOTA	1749 1750	SE	MSE	232 232	33.237	30.431	-2.467	1.00 52.07
ATOM	1751	C	MSE	232	34.286 29.694	30.483	-3.969	1.00 48.20
		0				30.664	-5.137	
ATOM ATOM	1752 1753	N	MSE	232 233	30.179 28.698	31 -656	-5.678 -5.668	1.00 36.84
ATOM	1754	CA	GLN	233	28.110	29.970 30.331	-6.948	1.00 38.35
ATOM	1755							1.00 40.19
ATOM	1756	CB	GLN GLN	233 233	26.954 25.658	29.373	-7.257 -7.672	1.00 40.19
ATOM	1757	CD	GLN	233	24.460	30.041 29.119	-7.510	1.00 41.80
ATOM	1758	OE1		233	24.226	28.582	-6.424	1.00 44.27
ATOM	1759	NE2		233	23.688	28.936	-8.586	1.00 43.87
ATOM	1760	C	GLN	233	27.615	31.777	-6.936	1.00 38.45
ATOM	1761	0	GLN	233	27.495	32.407	-7.984	1.00 39.07
ATOM	1762	N	ASN	234	27.329	32.407	-5.753	1.00 37.79
ATOM	1763	CA	ASN	234	26.840	33.687	-5.668	1.00 36.56
ATOM	1764	CB	ASN	234	25.657	33.771	-4.706	1.00 37.03
ATOM	1765	CG	ASN	234	24.505	32.864	-5.119	1.00 36.83
A 1 OH	1103		A SIV	234	24.303	32.004	-3.113	1.00 30.03

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ATOM	1766	ODI	ASN	234	24.152	32.793	-6.299	1.00 36.50
ATOM	1767		ASN	234				
					23.910	32.173	-4.146	1.00 36.25
MOTA	1768	C	ASN	234	27.919	34.676	-5.250	1.00 35.71
MOTA	1769	0	ASN	234	27.712	35.890	-5.301	1.00 35.11
MOTA	1770	N	VAL	235	29.069	34.156	-4.837	1.00 35.22
ATOM	1771	CA	VAL	235	30.177	35.009	-4.439	1.00 34.85
ATOM	1772	CB	VAL	235	31.056	34.321	-3.384	1.00 34.01
ATOM	1773	CG1		235	31.949	35.343	-2.717	1.00 32.35
MOTA	1774		VAL	235	30.185	33.576	-2.376	1.00 32.63
MOTA	1775	C	VAL	235	30.999	35.209	-5.706	1.00 35.79
MOTA	1776	0	VAL	235	32.011	34.548	-5.910	1.00 35.65
MOTA	1777	N	GLU	236	30.556	36.125	-6.556	1.00 37.55
MOTA	1778	CA	GLU	236	31.220	36.383	-7.830	1.00 39.52
MOTA	1779	CB	GLU	236	30.337	37.284	-8.701	1.00 39.67
ATOM	1780	CG	GLU	236	29.242	36.539	-9.448	1.00 41.02
ATOM	1781	CD	GLU	236	28.214	37.467	-10.072	1.00 42.58
ATOM	1782	OE1		236	28.607		-10.630	1.00 42.67
ATOM	1783	OE2		236	27.009	37.121	-10.011	1.00 43.02
ATOM	1784	c	GLU	236	32.631	36.961	-7.782	1.00 40.97
ATOM	1785	ō	GLU	236	33.328	36.967	-8.803	1.00 42.27
ATOM	1786	N	LEU	237	33.064	37.457	-6.628	1.00 41.32
ATOM	1787	CA	LEU	237	34.408	38.017	-6.538	1.00 41.63
ATOM	1788	CB	LEU	237	34.438	39.163	-5.537	1.00 41.68
ATOM	1789	CG	LEU	237	33.545			1.00 42.50
ATOM	1790		LEU	237	33.630	40.367	-5.820	
ATOM	1791		LEU	237	33.984	41.301	-4.623 -7.085	1.00 44.17
ATOM	1792	CD2	LEU	237	35.454			
ATOM	1793	0	LEU			36.970	-6.148	1.00 42.43
ATOM		N		237	36.636	37.294	-6.010	1.00 42.30
	1794		VAL	238	35.019	35.724	-5.967	1.00 42.96
ATOM	1795	CA	VAL	238	35.922	34.629	-5.606	1.00 43.89
ATOM	1796	CB	VAL	238	35.917	34.380	-4.097	1.00 42.33
MOTA	1797	CG1		238	36.722	33.136	-3.769	1.00 41.32
MOTA	1798	CG2		238	36.503	35.578	-3.385	1.00 42.74
MOTA	1799	C	VAL	238	35.520	33.337	-6.313	1.00 45.65
MOTA	1800	0	VAL	238	34.755	32.555	-5.770	1.00 46.15
MOTA	1801	N	GLU	239	36.069	33.116	-7.510	1.00 47.60
MOTA	1802	CA	GLU	239	35.769	31.947	-8.346	1.00 48.96
MOTA	1803	CB	GLU	239	36.819	31.793	-9.448	1.00 51.17
ATOM	1804	CG	GLU	239	37.000	33.026	-10.290	1.00 53.95
MOTA	1805	CD	GLU	239	37.817	34.066	-9.570	1.00 56.27
ATOM	1806	0E1		239	39.070	33.982	-9.637	1.00 58.40
ATOM	1807	OE2		239	37.211	34.950	-8.918	1.00 57.25
ATOM	1808	C	GLU	239	35.599	30.594	-7.675	1.00 48.87
MOTA	1809	0	GLU	239	36.272	30.274	-6.701	1.00 48.25
ATOM	1810	N	GLY	240	34.705	29.797	-8.252	1.00 49.09
ATOM	1811	CA	GLY	240	34.412	28.469	-7.750	1.00 50.05
ATOM	1812	C	GLY	240	32.967	28.418	-7.296	1.00 51.04
ATOM	1813	0	GLY	240	32.482	29.379	-6.712	1.00 52.00
MOTA	1814	N	ASP	241	32.259	27.332	-7.580	1.00 51.38
MOTA	1815	CA	ASP	241	30.882	27.214	-7.127	1.00 52.10
ATOM	1816	CB	ASP	241	29.963	26.766	-8.252	1.00 52.95
MOTA	1817	CG	ASP	241	30.186	27.534	-9.529	1.00 53.84
ATOM	1818	0D1	ASP	241	30.046	28.779	-9.522	1.00 53.20
ATOM	1819	OD2	ASP	241	30,496	26.875	-10.546	1.00 53.97
ATOM	1820	C	ASP	241	30.924	26.122	-6.083	1.00 52.90
ATOM	1821	0	ASP	241	29.898	25.563	-5.701	1.00 53.59
MOTA	1822	N	GLU	242	32.131	25.816	-5.626	1.00 53.45
ATOM	1823	CA	GLU	242	32.325	24.760	-4.646	1.00 53.65
ATOM	1824	CB	GLU	242	33.785	24.299	-4.670	1.00 55.19
					-333	24.233	4.070	

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ATOM	1825	CG	GLU	242	34.056	23.062	-3.826	1.00 57.57
ATOM	1826	CD	GLU	242	35.527	22.672	-3.811	1.00 58.85
ATOM	1827	OE1	GLU	242			-4.893	1.00 59.63
		OE2		242	36.063	22.340		1.00 59.85
ATOM	1828		GLU		36.143	22.701	-2.717	
ATOM	1829	C	GLU	242	31.933	25.159	-3.229	1.00 52.66
ATOM	1830	0	GLU	242	32.469	26.113	-2.661	1.00 53.15
ATOM	1,831	N	GLY	243	30.987	24.418	-2.665	1.00 51.11
MOTA	1832	CA	GLY	243	30.545	24.673	-1.305	1.00 48.74
MOTA	1833	C	GLY	243	30.200	26.110	-0.967	1.00 46.87
MOTA	1834	0	GLY	243	29.879	26.917	-1.850	1.00 46.49
ATOM	1835	N	ARG	244	30.288	26.421	0.326	1.00 44.89
ATOM	1836	CA	ARG	244	29.967	27.748	0.838	1.00 43.27
ATOM	1837	CB	ARG	244	28.852	27.639	1.873	1.00 42.24
ATOM	1838	CG	ARG	244	27.571	27.040	1.339	1.00 42.16
ATOM	1839	CD	ARG	244	26.442	27.153	2.356	1.00 41.35
MOTA	1840	NE	ARG	244	25.254	26.425	1.925	1.00 39.30
MOTA	1841	CZ	ARG	244	24.702	25.446	2.630	1.00 39.15
ATOM	1842	NH1	ARG	244	25.236	25.085	3.794	1.00 38.10
MOTA	1843	NH2	ARG	244	23.627	24.821	2.168	1.00 38.77
MOTA	1844	С	ARG	244	31.121	28.524	1.465	1.00 42.34
ATOM	1845	0	ARG	244	32.089	27.945	1.958	1.00 41.77
ATOM	1846	N	MSE	245	30.990	29.849	1.446	1.00 42.07
ATOM	1847	CA	MSE	245	31.977	30.745	2.042	1.00 41.32
ATOM	1848	CB	MSE	245	32.846	31.391	0.974	1.00 42.25
ATOM	1849	CG	MSE	245	33.870	32.345	1.566	1.00 44.07
ATOM	1850	SE	MSE	245	34.884	33.206	0.332	1.00 47.16
MOTA	1851	CE	MSE	245	36.149	31.909	-0.005	1.00 44.40
MOTA	1852	С	MSE	245	31.324	31.863	2.863	1.00 40.37
ATOM	1853	Ö	MSE	245	30.525	32.644	2.338	1.00 40.13
MOTA	1854	N	CYS	246	31.664	31.940	4.148	1.00 38.95
ATOM	1855	CA	CYS	246	31.125	32.990	5.001	1.00 37.00
ATOM	1856	CB	CYS	246	31.794	32.953	6.376	1.00 37.69
ATOM	1857	SG	CYS	246	31.231	34.229	7.567	1.00 38.96
ATOM	1858	c	CYS	246	31.422	34.320	4.311	1.00 35.82
ATOM	1859	ō	CYS	246	32.484	34.497	3.706	1.00 34.54
ATOM	1860	N	VAL	247	30.466	35.240	4.388	1.00 34.51
ATOM	1861	CA	VAL	247	30.591	36.566	3.782	1.00 32.46
ATOM	1862	CB	VAL	247	29.609	36.751	2.588	1.00 32.34
ATOM	1863		VAL	247	29.709	38.170	2.038	1.00 31.78
ATOM	1864		VAL	247	29.930	35.750	1.486	1.00 32.04
ATOM	1865	c	VAL	247	30.239	37.580	4.863	1.00 32.03
ATOM	1866	ō	VAL	247	29.291	37.377	5.628	1.00 33.28
ATOM	1867	N	ASN	248	31.011	38.657	4.931	1.00 29.34
ATOM	1868	CA	ASN	248	30.792	39.699	5.917	1.00 27.36
ATOM	1869	CB	ASN	248	32.147	40.219	6.401	1.00 28.42
ATOM	1870	CG	ASN	248	32.031	41 -471	7.253	1.00 29.34
ATOM	1871	0D1		248	30.975	41.774	7.816	1.00 29.82
ATOM	1872		ASN	248	33.141	42.201	7.374	1.00 29.54
ATOM	1873	C	ASN	248	29.983	40.798	5.257	1.00 27.10
ATOM	1874	ō	ASN	248	30.531	41.618	4.503	1.00 26.98
ATOM	1875	N	THR	249	28.679	40.823	5.544	1.00 26.01
ATOM	1876	CA	THR	249	27.778	41.809	4.937	1.00 23.85
ATOM	1877	CB	THR	249	26.325	41.634	5.424	1.00 23.83
ATOM	1878	0G1		249	26.228	42.100	6.775	1.00 25.01
ATOM	1879	CG2		249	25.899		5.380	1.00 22.15
ATOM	1880	C	THR	249	28.208	40.156 43.226	5.270	1.00 24.20
ATOM	1881	0	THR	249	28.023	44.143	4.467	1.00 23.38
ATOM	1882	N	GLU	250	28.023	44.143	6.462	1.00 24.31
	1883	CA	GLU	250	29.219	44.733	6.891	1.00 24.31
MOTA	1983	CA	GLU	230	29.219	44./33	0.891	1.00 23.61

Figur 4

1	igur 4							
	1004	O.D.		0.50				
ATOM	1884	CB	GLU	250	30.446	45.145	6.060	1.00 23.87
ATOM	1885	CG	GLU	250	31.242	46.362	6.571	1.00 25.94
ATOM	1886	CD	GLU	250	32.237	46.041	7.700	1.00 25.83
ATOM	1887	OE1	GLU	250	32.728	44.893	7.813	1.00 25.67
ATOM	1888		GLU	250	32.552	46.960	8.473	1.00 26.46
MOTA	1889	С	GLU	250	28.003	45.624	6.589	1.00 23.30
MOTA	1890	0	GLU	250	28.110	46.648	5.896	1.00 23.33
MOTA	1891	N	TRP	251	26.841	45.208	7.096	1.00 22.28
MOTA	1892	CA	TRP	251	25.609	45.940	6.840	1.00 22.36
MOTA	1893	CB	TRP	251	24.376	45.077	7.133	1.00 20.65
MOTA	1894	CG	TRP	251	24.133	44.726	8.543	1.00 18.29
MOTA	1895	CD2	TRP	251	23.308	43.648	9.016	1.00 16.51
ATOM	1896	CE2	TRP	251	23.279	43.725	10.424	1.00 15.08
ATOM	1897	CE3	TRP	251	22.589	42.635	8.384	1.00 16.17
MOTA	1898	CD1	TRP	251	24.565	45.395	9.652	1.00 17.71
MOTA	1899	NE1	TRP	251	24.051	44.795	10.795	1.00 17.10
MOTA	1900	CZ2	TRP	251	22.567	42.830	11.201	1.00 14.23
ATOM	1901	CZ3	TRP	251	21.872	41.737	9.171	1.00 15.72
MOTA	1902	CH2	TRP	251	21.869	41.842	10.559	1.00 14.23
MOTA	1903	С	TRP	251	25.445	47.283	7.523	1.00 23.49
MOTA	1904	0	TRP	251	24.541	48.044	7.167	1.00 23.95
ATOM	1905	N	GLY	252	26.302	47.579	8.500	1.00 24.44
MOTA	1906	CA	GLY	252	26.214	48.857	9.179	1.00 25.17
MOTA	1907	C	GLY	252	26.195	49.979	8.152	1.00 26.19
MOTA	1908	0	GLY	252	25.715	51.086	8.429	1.00 26.19
MOTA	1909	N	ALA	253	26.714	49.675	6.960	1.00 26.83
MOTA	1910	CA	ALA	253	26.791	50.622	5.851	1.00 27.86
ATOM	1911	CB	ALA	253	27.822	50.148	4.851	1.00 27.90
MOTA	1912	С	ALA	253	25.448	50.834	5.144	1.00 28.52
ATOM	1913	0	ALA	253	25.249	51.834	4.448	1.00 27.73
ATCM	1914	N	PHE	254	24.536	49.884	5.314	1.00 30.23
MOTA	1915	CA	PHE	254	23.224	49.974	4.696	1.00 31.42
ATOM	1916	CB	PHE	254	22.289	48.947	5.314	1.00 31.71
MOTA	1917	CG	PHE	254	20.899	48.995	4.768	1.00 31.90
ATOM	1918	CD1	PHE	254	20.655	48.736	3.429	1.00 31.47
ATOM	1919	CD2	PHE	254	19.824	49.273	5.600	1.00 32.95
MOTA	1920	CE1	PHE	254	19.367	48.746	2.927	1.00 31.38
MOTA	1921	CE2	PHE	254	18.518	49.285	5.096	1.00 32.69
ATOM	1922	CZ	PHE	254	18.295	49.021	3.763	1.00 31.47
MOTA	1923	С	PHE	254	22.664	51.367	4.928	1.00 32.56
MOTA	1924	0	PHE	254	22.638	51.839	6.064	1.00 33.19
ATOM	1925	N	GLY	255	22.227	52.017	3.849	1.00 33.62
ATOM	1926	CA	GLY	255	21.674	53.354	3.947	1.00 34.98
ATOM	1927	С	GLY	255	22.673	54.429	3.565	1.00 36.85
ATOM	1928	0	GLY	255	22.317	55.604	3.424	1.00 36.70
ATOM	1929	N	ASP	256	23.932	54_038	3.395	1.00 38.95
MOTA	1930	CA	ASP	256	24.966	55.000	3.038	1.00 41.47
ATOM	1931	CB	ASP	256	26.349	54.347	3.088	1.00 41.77
MOTA	1932	CG	ASP	256	26.880	54.224	4.502	1.00 42.36
ATOM	1933	OD1		256	26.573	55.120	5.322	1.00 43.08
ATOM	1934	OD2		256	27.617	53.251	4.791	1.00 42.28
MOTA	1935	С	ASP	256	24.744	55.636	1.666	1.00 43.10
MOTA	1936	0	ASP	256	25.489	56.533	1.261	1.00 44.08
ATOM	1937	N	SER	257	23.729	55.171	0.946	1.00 44.19
MOTA	1938	CA	SER	257	23.427	55.738	-0.363	1.00 45.32
ATOM	1939	CB	SER	257	23.714	54.713	-1.467	1.00 45.78
MOTA	1940	OG	SER	257	22.845	53.601	-1.375	1.00 46.48
MOTA	1941	C	SER	257	21.967	56.204	-0.423	1.00 45.41
ATOM	1942	0	SER	257	21.378	56.316	-1.501	1.00 46.14

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ATOM	1943	N	GLY	258	21.393	56.466	0.751	1.00 45.52
ATOM	1944	CA	GLY	258	20.018	56.933	0.835	1.00 45.22
ATOM	1945	C	GLY	258	18.922	55.896	1.042	1.00 45.11
ATOM	1946	ō	GLY	258	17.745	56.253	1.068	1.00 45.45
ATOM	1947	N	GLU	259	19.284	54.627	1.205	1.00 44.67
ATOM	1948	CA	GLU	259	18.288	53.572	1.380	1.00 44.04
ATOM	1949	CB	GLU	259	18.954	52.187	1.415	1.00 44.23
ATOM	1950	CG	GLU	259	19.952	51.916	0.295	1.00 44.88
ATOM	1951	CD	GLU	259	21.318	52.552	0.548	1.00 45.53
ATOM	1952	OE1		259	21.381	53.785	0.753	1.00 44.98
MOTA	1953		GLU	259	22.335	51.817	0.733	1.00 45.95
ATOM	1954	C	GLU	259	17.462	53.749	2.647	1.00 43.91
ATOM	1955	ō	GLU	259	16.461	53.061	2.836	1.00 43.49
MOTA	1956	N	LEU	260	17.875	54.661	3.520	1.00 43.49
ATOM	1957	CA	LEU	260	17.143	54.865	4.765	1.00 44.40
ATOM	1958	CB	LEU	260	18.023	54.513	5.967	1.00 44.36
ATOM	1959	CG	LEU	260	18.398	53.041	6.153	1.00 44.87
ATOM	1960		LEU	260	19.315	52.879	7.369	1.00 44.30
ATOM	1961		LEU	260	17.127	52.216	6.307	1.00 44.88
ATOM	1962	C	LEU	260	16.632	56.282	4.932	1.00 44.59
ATOM	1963	0	LEU	260	15.744	56.534	5.749	1.00 44.72
ATOM	1964	N	ASP	261	17.200	57.202	4.161	1.00 44.72
ATOM	1965	CA	ASP	261	16.821	58.608	4.234	1.00 44.48
ATOM	1966	CB	ASP	261	16.813	59.224	2.841	1.00 44.18
ATOM	1967	CG	ASP	261	18.192	59.310	2.247	1.00 45.23
ATOM	1968		ASP	261	19.165	58.994	2.247	1.00 45.23
ATOM	1969		ASP	261	18.296	59.697	1.055	1.00 46.42
ATOM	1970	C	ASP	261	15.482	58.885	4.892	1.00 43.00
MOTA	1971	ō	ASP	261	15.415	59.592	5.898	1.00 42.63
ATOM	1972	N	GLU	262	14.424	58.317	4.320	1.00 41.88
ATOM	1973	CA	GLU	262	13.070	58.525	4.810	1.00 41.00
ATOM	1974	CB	GLU	262	12.088	57.744	3.940	1.00 41.65
ATOM	1975	CG	GLU	262	12.249	56.254	3.999	1.00 43.54
MOTA	1976	CD	GLU	262	11.359	55.562	2.996	1.00 45.44
ATOM	1977	OE1	GLU	262	11.715	55.561	1.800	1.00 47.21
ATOM	1978	OE2	GLU	262	10.296	55.031	3.391	1.00 47.29
ATOM	1979	C	GLU	262	12.830	58.211	6.286	1.00 39.99
MOTA	1980	0	GLU	262	11.997	58.852	6.918	1.00 40.22
ATOM	1981	M	PHE	263	13.545	57.238	6.845	1.00 38.83
ATOM	1932	CA	PHE	263	13.360	56.908	8.258	1.00 37.00
ATOM	1983	CB	PHE	263	13.684	55.430	8.512	1.00 34.37
ATOM	1984	CG	PHE	263	12.828	54.476	7.717	1.00 32.41
MOTA	1985	CD1		263	13.366	53.753	6.660	1.00 30.67
ATOM	1986	CD2		263	11.474	54.317	8.012	1.00 30.95
ATOM	1987	CE1		263	12.567	52.886	5.909	1.00 29.82
ATOM	1988	CE2		263	10.667	53 .450	7.261	1.00 28.87
ATOM	1989	CZ	PHE	263	11.214	52.737	6.213	1.00 29.09
ATOM	1990	C	PHE	263	14.197	57.797	9.190	1.00 36.78
ATOM	1991	0	PHE	263	13.809	58.041	10.327	1.00 37.58
ATOM	1992	N	LEU	264	15.328	58.301	8.712	1.00 36.72
ATOM	1993	CA	LEU	264	16.193	59.142	9.542	1.00 37.11
ATOM	1994	CB	LEU	264	17.389	59.638	8.725	1.00 36.98
ATOM	1995	CG	LEU	264	18.131	58.621	7.852	1.00 36.59
MOTA	1996 1997		LEU	264	19.233	59.346	7.077	1.00 35.39
ATOM	1997	CD2	LEU	264 264	18.701 15.482	57.503	8.717	1.00 35.46 1.00 37.28
ATOM	1998	0	LEU	264	15.482	60.350 61.148	9.451	1.00 37.28
ATOM	2000	N	LEU	265	15.574	60.480	11.479	1.00 38.03
ATOM	2001	CA	LEU	265	14.965	61.585	12.215	1.00 37.03
VION	2001	CA	шьо	203	14.703	01.565	12.213	1.00 37.33

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Figur 4

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ATOM	2002	CB	T DIT	265	14 200	61 070	12 522	1 00 26 25
			LEU		14.380	61.070	13.527	1.00 36.25
MOTA	2003	CG	LEU	265	13.529	59.807	13.417	1.00 35.76
MOTA	2004	CD1	LEU	265	13.157	59.295	14.808	1.00 35.17
MOTA	2005	CE2	LEU	265	12.292	60.120	12.598	1.00 35.59
MOTA	2006	C	LEU	265	16.054	62.613	12.521	1.00 38.22
ATOM	2007	0	LEU	265	17.239	62.285	12.486	1.00 38.34
MOTA	2008	N	GLU	266	15.653	63.844	12.832	1.00 39.22
ATOM	2009	CA	GLU	266	16.599	64.922	13.137	1.00 40.56
ATOM	2010	CB	GLU	266	15.874	66.101	13.813	1.00 41.82
MOTA	2011	CG	GLU	266	15.277	65.777	15.196	1.00 44.28
MOTA	2012	CD	GLU	266	14.612	66.974	15.886	1.00 44.95
MOTA	2013	OE1	GLU	266	13.543	67.432	15.410	1.00 45.08
MOTA	2014	OE2	GLU	266	15.163	67.452	16.910	1.00 45.53
MOTA	2015	C	GLU	266	17.733	64.435	14.036	1.00 40.54
ATOM	2016	0	GLU	266	18.910	64.657	13.750	1.00 40.69
ATOM	2017	N	TYR	267	17.366	63.760	15.121	1.00 40.61
ATOM	2018	CA	TYR	267	18.342	63.234	16.062	1.00 40.30
ATOM	2019	CB	TYR	267	17.639	62.364	17.110	1.00 39.44
ATOM	2020	CG	TYR	267	16.216	62.784	17.423	1.00 38.98
ATOM	2021	CD1		267	15.134	61.967	17.066	1.00 38.66
ATOM	2022	CE1	TYR	267	13.813	62.342	17.349	1.00 38.28
ATOM	2023	CD2		267	15.943	63.995	18.075	1.00 38.72
ATOM	2024	CE2	TYR	267	14.619	64.381	18.364	1.00 38.45
ATOM	2025	CZ	TYR	267	13.564	63.548	17.996	1.00 38.30
MOTA	2026	OH	TYR	267	12.267	63.923	18.251	1.00 37.22
ATOM	2027	C.	TYR	267	19.381	62.403	15.296	1.00 40.27
MOTA	2028	ō	TYR	267	20.580	62.469	15.579	1.00 40.14
ATOM	2029	N	ASP	268	18.909	61.626	14.324	1.00 40.61
MOTA	2030	CA	ASP	268	19.781	60.790	13.511	1.00 40.87
ATOM	.2031	CB	ASP	268	18.946	59.920	12.566	1.00 39.36
MOTA	2032	CG	ASP	268	18.183	58.843	13.301	1.00 38.52
ATOM	2032		ASP	268	18.819			1.00 30.32
ATOM	2033		ASP	268	16.961	58.118	14.082	1.00 36.13
ATOM	2035	C	ASP	268	20.764	58.711	13.110	
ATOM	2036	0	ASP	268	21.956	61.643	12.712	1.00 41.97
ATOM	2037	N	ARG	269	20.266	61.339	12.667	
ATOM	2037	CA				62.710	12.090	1.00 42.73
ATOM	2038	CB	ARG	269	21.113	63.606	11.310	1.00 43.23
ATOM	2039		ARG	269	20.302	64.793	10.786	1.00 45.34
ATOM	2040	CG	ARG	269	18.923	64.464	10.223	1.00 47.46
ATOM	2041	NE	ARG	269 269	19.000	63.819	8.864	1.00 49.22
ATOM	2042	CZ	ARG		17.667	63.552	8.337	1.00 52.67
ATOM	2043	NH1		269 269	17.426	62.969	7.165	1.00 54.63
MOTA		NH1			18.436	62.591	6.386	1.00 55.41
ATOM	2045 2046	C		269 269	16.173	62.747	6, 775	1.00 55.38
			ARG		22.204	64.150	12.231	1.00 42.99
ATOM	2047	0	ARG	269	23.400	63 .999	11.977	1.00 43.63
ATOM	2048	N	LEU	270	21.777	64.796	13.305	1.00 41.99
ATOM	2049	CA	LEU	270	22.702	65.372	14.261	1.00 41.33
ATOM	2050	CB	LEU	270	21.924	65.812	15.502	1.00 41.15
ATOM	2051	CG	LEU	270	21.004	67.002	15.217	1.00 40.34
ATOM	2052	CD1		270	19.964	67.182	16.307	1.00 39.94
ATOM	2053	CD2		270	21.879	68.237	15.084	1.00 40.26
ATOM	2054	С	LEU	270	23.828	64.406	14.635	1.00 41.26
ATOM	2055	0	LEU	270	25.009	64.762	14.553	1.00 41.76
ATOM	2056	N	VAL	271	23.462	63.188	15.030	1.00 40.24
ATOM	2057	CA	VAL	271	24.443	62.177	15.415	1.00 40.08
ATOM	2058	CB	VAL	271	23.776	60.838	15.730	1.00 40.42
MOTA	2059		VAL	271	24.846	59.800	16.050	1.00 39.86
MOTA	2060	CG2	VAL	271	22.796	61.000	16.891	1.00 40.86

Figur 4

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ATOM	2061		VAL	271	25.477	61 000	14 200	1.00 40.51
ATOM	2061 2062	0		271	26.676	61.903	14.329	
		N	VAL	272		61.832	14.595	1.00 40.15 1.00 40.78
MOTA MOTA	2063 2064	CA	ASP	272	24.998 25.866	61.730	13.103 11.977	1.00 40.78
		CB	ASP	272		61.447		
ATOM	2065	CG			25.038	61.344	10.695	1.00 39.16
MOTA	2066		ASP	272	25.792	60.670	9.553	1.00 38.09
MOTA	2067	ODI		272	26.821	60.000	9.807	1.00 36.54
ATOM	2068	OD2	ASP	272	25.335	60.798	8.394	1.00 37.12
ATOM	2069	C	ASP	272	26.901	62.544	11.849	1.00 40.88
MOTA	2070	0	ASP	272	28.099	62.297	11.953	1.00 40.75
ATOM	2071	N	GLU	273	26.429	63.763	11.638	1.00 41.96
ATOM	2072	CA	GLU	273	27.321	64.896	11.477	1.00 43.14
ATOM	2073	CB	GLU	273	26.501	66.170	11.470	1.00 44.13
MOTA	2074	CD	GLU	273 273	25.576	66.214	10.272	1.00 46.73
ATOM	2075		GLU		24.629	67.388	10.308	
ATOM	2076	OE2	GLU	273 273	25.047 23.482	68.455	10.828	1.00 49.15
ATOM	2077		GLU	273		67.241	9.811	1.00 48.64
MOTA	2078	С		273	28.428	64.968	12.517	
MOTA	2079	0	GLU	274	29.575 28.095	65.279	12.187	1.00 43.59
ATOM	2080	N CA	SER	2.74	29.089	64.666 64.702	13.767 14.837	1.00 44.54
ATOM ATOM	2081	CB	SER	274	28.421	64.762	16.205	1.00 45.39
ATOM	2083	OG	SER	274	27.496	65.611	16.424	1.00 48.14
ATOM	2084	C	SER	274	30.106	63.582	14.694	1.00 44.23
ATOM	2085	0	SER	274	31.292	63.783	14.034	1.00 44.76
ATOM	2086	N	SER	275	29.632	62.400	14.318	1.00 43.84
ATOM	2087	CA	SER	275	30.489	61.227	14.162	1.00 43.42
ATOM	2088	CB	SER	275	29.754	60.139	13.392	1.00 43.28
ATOM	2089	OG	SER	275	29.758	60.444	12.010	1.00 42.94
ATOM	2090	C	SER	275	31.789	61.535	13.426	1.00 43.34
MOTA	2091	ō	SER	275	31.914	62.552	12.738	1.00 43.76
ATOM	2092	N	ALA	276	32.756	60.639	13.570	1.00 42.68
ATOM	2093	CA	ALA	276	34.034	60.805	12.906	1.00 42.98
ATOM	2094	CB	ALA	276	35.108	60.015	13.639	1.00 42.92
ATOM	2095	C	ALA	276	33.930	60.319	11.465	1.00 43.23
ATOM	2096	0	ALA	276	34.936	60.277	10.751	1.00 44.60
ATOM	2097	N	ASN	277	32.722	59.949	11.039	1.00 42.10
ATOM	2098	CA	ÁSN	277	32.517	59.447	9.691	1.00 40.87
MOTA	2099	ÇB	ASN	277	32.615	57.927	9.685	1.00 41.63
MOTA	2100	CG	ASN	277	31.654	57.283	10.659	1.00 42.64
MOTA	2101		ASN	277	30.670	57.898	11.067	1.00 43.50
ATOM	2102	ND2		277	31.925	56.033	11.029	1.00 42.98
MOTA	2103	C	ASN	277	31.178	59.865	9.104	1.00 40.57
ATOM	2104	0	ASN	277	30.430	59.039	8.579	1.00 39.89
ATOM	2105	N	PRO	278	30.868	61.163	9.163	1.00 40.83
ATOM	2106 2107	CD	PRO	278 278	31.783	62 . 282	9.451	1.00 40.71
ATOM ATOM	2107	CA	PRO	278	29.600 29.807	61.657 63.175	8.623 8.579	1.00 40.71
ATOM	2109	CG	PRO	278	31.303	63.326	8.474	1.00 41.27
ATOM	2110	c	PRO	278	29.239	61.074	7.258	1.00 40.60
ATOM	2111	ō	PRO	278	29.949	61.284	6.270	1.00 40.71
ATOM	2112	N	GLY	279	28.131	60.338	7.216	1.00 40.34
ATOM	2113	CA	GLY	279	27.676	59.747	5.971	1.00 39.10
ATOM	2114	C	GLY	279	27.904	58.252	5.828	1.00 38.94
ATOM	2115	ō	GLY	279	27.315	57.635	4.952	1.00 39.74
ATOM	2116	N	GLN	280	28.735	57.660	6.683	1.00 38.66
ATOM	2117	CA	GLN	280	29.049	56.230	6.605	1.00 37.75
ATOM	2118	CB	GLN	280	30.563	56.043	6.513	1.00 37.97
ATOM	2119	CG	GLN	280	31.243	56.954	5.509	1.00 39.85

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ATOM	2120	CD	GLN	280	32.743	57.046	E 720	1 00 10 76
							5.730	1.00 40.76
MOTA	2121	OE1	GLN	280	33.465	56.058	5.587	1.00 41.39
ATOM	2122	NE2	GLN	280	33.220	58.240	6.083	1.00 41.57
MOTA	2123	C	GLN	280	28.553	55.455	7.817	1.00 36.99
ATOM	2124	0	GLN	280	28.645	55.939	8.941	1.00 37.89
ATOM	2125	N	GLN	281	28.054	54.242	7.592	1.00 35.75
ATOM	2126	CA	GLN	281	27.572	53.401	8.681	1.00 34.04
ATOM	2127	CB	GLN	281	28.590	53,404	9.829	1.00 33.35
ATOM	2128	CG	GLN	281	29.971	52.951	9.447	1.00 33.09
ATOM	2129	CD	GLN	281	29.967	51.576	8.800	1.00 34.44
ATOM	2130	OE1	GLN	281	29.917	51.451	7.572	1.00 34.44
ATOM	2131	NE2	GLN	281				
					30.000	50.529	9.630	1.00 34.63
MOTA	2132	C	GLN	281	26.210	53.831	9.237	1.00 33.42
ATOM	2133	0	GLN	281	25.895	53.530	10.390	1.00 34.87
ATOM	2134	N	LEU	282	25.395	54.511	8.436	1.00 31.53
MOTA	2135	CA	LEU	282	24.098	54.992	8.913	1.00 29.87
ATOM	2136	CB	LEU	282	23.345	55.685	7.777	1.00 30.15
ATOM	2137	CG	LEU	282	24.030	56.871	7.085	1.00 30.41
ATOM	2138	CD1	LEU	282	22.963	57.741	6.435	1.00 29.82
MOTA	2139	CD2	LEU	282	24.815	57.699	8.097	1.00 30.66
ATOM	2140	C	LEU	282	23.191	53.949	9.578	1.00 28.70
ATOM	2141	ō	LEU	282	22.716	54.153	10.698	1.00 28.78
ATOM	2142	N	TYR	283	22.935	52.841	8.894	1.00 27.35
ATOM	2143	CA	TYR	283				
					22.095	51.793	9.461	1.00 26.53
MOTA	2144	CB	TYR	283	22.233	50.511	8.633	1.00 24.41
ATOM	2145	CG	TYR	283	21.420	49.338	9.143	1.00 22.90
MOTA	2146	CD1		283	20.021	49.413	9.210	1.00 21.94
ATOM	2147		TYR	283	19.257	48.318	9.609	1.00 20.96
ATOM	2148	CD2		283	22.038	48.129	9.503	1.00 21.53
ATOM	2149	CE2	TYR	283	21.279	47.030	9.907	1.00 20.87
ATOM '	2150	CZ	TYR	283	19.886	47.140	9.950	1.00 21.33
MOTA	2151	OH	TYR	283	19.105	46.068	10.310	1.00 23.85
ATOM	2152	C	TYR	283	22.567	51.532	10.891	1.00 27.12
MOTA	2153	0	TYR	283	21.783	51.521	11.841	1.00 28.95
ATOM	2154	N	GLU	284	23.869	51.352	11.035	1.00 26.60
MOTA	2155	CA	GLU	284	24.486	51.072	12.317	1.00 26.43
ATOM	2156	CB	GLU	284	25.982	50.905	12.108	1.00 27.03
ATOM	2157	CG	GLU	284	26.763	50.680	13.375	1.00 27.03
MOTA	2158	CD	GLU	284	28.224	50.492	13.082	1.00 27.27
ATOM	2159	OE1		284	28.897			
						51.506	12.734	1.00 27.02
ATOM	2160	OE2		284	28.670	49.319	13.185	1.00 26.30
MOTA	2161	C	GLU	284	24.249	52.133	13.381	1.00 26.81
MOTA	2162	0	GLU	284	24.197	51.826	14.582	1.00 26.06
ATOM	2163	N	LYS	285	24.134	53.384	12.940	1.00 27.07
ATOM	2164	CA	LYS	285	23.926	54.502	13.860	1.00 27.39
ATOM	2165	CB	LYS	285	24.339	55 -825	13.186	1.00 25.99
MOTA	2166	CG	LYS	285	25.840	56.012	13.132	1.00 24.13
ATOM	2167	CD	LYS	285 -	26.235	57.110	12.179	1.00 23.29
ATOM	2168	CE	LYS	285	27.755	57.193	12.052	1.00 22.03
ATOM	2169	NZ	LYS	285	28.142	58.198	11.027	1.00 21.72
ATOM	2170	C	LYS	285	22.488	54.595	14.368	1.00 28.05
ATOM	2171	ō	LYS	285	22.086	55.615	14.941	1.00 28.61
ATOM	2172	N	LEU	286	21.717	53.535	14.144	1.00 27.60
ATOM	2173	CA	LEU	286				
					20.335	53.488	14.599	1.00 27.30
ATOM	2174	CB	LEU	286	19.399	53.157	13.435	1.00 28.57
ATOM	2175	CG	LEU	286	19.375	54.167	12.279	1.00 30.25
MOTA	2176	CD1		286	18.480	53.647	11.139	1.00 29.98
ATOM	2177		LEU	286	18.863	55.507	12.780	1.00 29.35
MOTA	2178	С	LEU	286	20.260	52.381	15.632	1.00 27.01

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ATOM	2179	0	LEU	286	10 006			
ATOM	2180	N			19.296	52.294	16.399	1.00 27.55
			ILE	287	21.306	51.554	15.645	1.00 26.00
MOTA	2181	CA	ILE	287	21.415	50.399	16.532	1.00 24.38
ATOM	2182	CB	ILE	287	21.551	49.141	15.715	1.00 23.92
ATOM	2183	CG2	ILE	287	21.470	47.919	16.628	1.00 22.70
ATOM	2184	CG1	ILE	287	20.510	49.158	14.597	1.00 22.87
ATOM	2185	CD1	ILE	287	20.676	48.042	13.607	1.00 22.79
ATOM	2186	C	ILE	287	22.639	50.444	17.433	1.00 24.65
MOTA	2187	0	ILE	287	22.550	50.255	18.644	1.00 23.54
ATOM	2188	N	GLY	288	23.791	50.668	16.810	1.00 25.94
MOTA	2189	CA	GLY	288	25.060	50.714	17.519	1.00 26.86
ATOM	2190	C	GLY	288	25.081	51.266	18.927	1.00 27.76
MOTA	2191	0	GLY	288	24.697	52.412	19.164	1.00 28.19
MOTA	2192	M	GLY	289	25.554	50.445	19.860	1.00 28.95
MOTA	2193	CA	GLY	289	25.656	50.856	21.249	1.00 30.64
MOTA	2194	C	GLY	289	26.632	52.007	21.407	1.00 31.92
ATOM	2195	0	GLY	289	26.930	52.442	22.509	1.00 32.56
MOTA	2196	N	LYS	290	27.133	52.504	20.291	1.00 32.83
ATOM	2197	CA	LYS	290	28.067	53.607	20.296	1.00 33.99
MOTA	2198	CB	LYS	290	29.104	53.373	19.191	1.00 35.04
MOTA	2199	CG	LYS	290	29.858	54.598	18.665	1.00 36.71
ATOM	2200	CD	LYS	290	31.032	54.996	19.551	1.00 38.80
ATOM	2201	CE	LYS	290	31.936	56.011	18.839	1.00 39.77
ATOM	2202	NZ	LYS	290	32.864	56.707	19.787	1.00 41.04
ATOM	2203	C	LYS	290	27.278	54.880	20.035	1.00 34.58
ATOM	2204	0	LYS	290	27.810	55.984	20.138	1.00 35.79
ATOM	2205	N	TYR	291	26.001	54.734	19.708	1.00 33.80
ATOM	2206	CA	TYR	291	25.196	55.907	19.406	1.00 33.61
ATOM	2207	CB	TYR	291	25.010	56.046	17.892	1.00 33.22
ATOM	2208	CG	TYR	291	26.256	55.752	17.084	1.00 33.77
ATOM	2209	CD1	TYR	291	26.659	54.435	16.838	1.00 34.23
ATOM	2210	CE1	TYR	291	27.789	54.155	16.065	1.00 34.17
ATOM	2211	CD2	TYR	291	27.021	56.783	16.542	1.00 33.61
ATOM	2212	CE2	TYR	291	28.150	56.515	15.773	1.00 33.54
ATOM	2213	CZ	TYR	291	28.528	55.200	15.532	1.00 33.76
ATOM	2214	OH	TYR	291	29.620	54.928	14.729	1.00 34.36
ATOM	2215	C	TYR	291	23.836	55.874	20.070	1.00 33.11
ATOM	2216	0	TYR	291	23.069	56.828	19.975	1.00 32.86
ATOM	2217	N	MSE	292	23.521	54.778	20.737	1.00 33.27
ATOM	2218	CA	MSE	292	22.230	54.699	21.389	1.00 33.18
ATOM	2219	CB	MSE	292	22.066	53.349	22.062	1.00 33.77
MOTA	2220	CG	MSE	292	20.639	52.975	22.314	1.00 35.15
ATOM	2221	SE	MSE	292	20.564	51.230	22.803	1.00 41.54
ATOM	2222	CE	MSE	292	20.269	50.385	21.171	1.00 35.91
ATOM	2223	С	MSE	292	22.148	55.818	22.423	1.00 32.97
ATOM	2224	0	MSE	292	21.227	56637	22.400	1.00 33.49
ATOM	2225	N	GLY	293	23.131	55.861	23.315	1.00 32.96
ATOM	2226	CA	GLY	293	23.151	56.892	24.334	1.00 32.25
ATOM	2227	C	GLY	293	23.067	58.290	23.750	1.00 32.18
ATOM	2223	0	GLY	293	22.307	59.126	24.241	1.00 33.24
ATOM	2229	N	GLU	294	23.835	58.560	22.702	1.00 31.47
ATOM	2230	CA	GLU	294	23.809	59.883	22.096	1.00 31.38
ATOM	2231	CB	GLU	294	24.875	59.971	21.008	1.00 33.29
ATOM	2232	CG	GLU	294	24.986	61.321	20.304	1.00 34.67
ATOM	2233	CD	GLU	294	25.227	62.474	21.257	1.00 35.80
ATOM	2234	OE1		294	25.708	62.244	22.389	1.00 36.49
ATOM	2235	OE2	GLU	294	24.946	63.623	20.858	1.00 37.16
ATOM	2236	C	GLU	294	22.428	60.192	21.521	1.00 30.62
ATOM	2237	ō	GLU	294	21.919	61.305	21.664	1.00 30.94
		-				01.303	21.004	1.00 30.34

Figur 4

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MOTA	2238	N	LEU	295	21.818	59.204	20.878	1.00 29.56
ATOM	2239	CA	LEU	295	20.495	59.392	20.303	1.00 29.24
ATOM	2240	CB	LEU	295	20.030	58.112	19.589	1.00 27.27
MOTA	2241	CG	LEU	295	20.389	58.007	18.099	1.00 25.46
ATOM	2242	CD1	LEU	295	19.979	56.668	17.522	1.00 21.87
MOTA	2243	CD2	LEU	295	19.677	59.136	17.352	1.00 25.71
ATOM	2244	С	LEU	295	19.497	59.787	21.388	1.00 29.98
ATOM	2245	ō	LEU	295	18.587	60.573	21.156	1.00 30.19
ATOM	2246	N	VAL	296	19.665			
ATOM	2247	CA	VAL	296		59.250	22.585	1.00 31.23
					18.745	59.590	23.657	1.00 32.87
MOTA	2248	CB	VAL	296	18.890	58.623	24.831	1.00 32.48
MOTA	2249	CG1		296	17.827	58.899	25.868	1.00 32.99
MOTA	2250		VAL	296	18.762	57.198	24.323	1.00 33.56
ATOM	2251	C	VAL	296	19.020	61.025	24.122	1.00 33.74
ATOM	2252	0	VAL	296	18.086	61.778	24.431	1.00 33.68
ATOM	2253	N	ARG	297	20.296	61.409	24.145	1.00 34.02
ATOM	2254	CA	ARG	297	20.659	62.757	24.563	1.00 35.34
MOTA	2255	CB	ARG	297	22.147	63.008	24.342	1.00 34.89
ATOM	2256	CG	ARG	297	22.940	63.279	25.609	1.00 35.27
ATOM	2257	CD	ARG	297	23.791	64.525		1.00 35.27
ATOM	2258		ARG	297			25.454	
		NE			24.226	64.700	24.074	1.00 37.11
MOTA	2259	CZ	ARG	297	24.476	65.878	23.513	1.00 37.43
MOTA	2260	NH1		297	24.348	65.994	24.226	1.00 38.45
ATOM	2261	NH2	ARG	297	24.809	65.944	22.229	1.00 36.61
MOTA	2262	C	ARG	297	19.870	63.766	23.747	1.00 36.07
ATOM	2263	0	ARG	297	19.103	64.574	24.285	1.00 36.76
ATOM	2264	N	LEU	298	20.063	63.699	22.437	1.00 36.93
ATOM	2265	CA	LEU	298	19.407	64.596	21.500	1.00 37.55
ATOM	2266	CB	LEU	298	19.768	64.178	20.077	1.00 37.28
ATOM	2267	CG	LEU	298	21.272	64.065	19.816	1.00 36.13
ATOM	2268		LEU	298	21.478	63.784	18.341	1.00 36.85
ATOM	2269		LEU	298	21.991	65.356	20.218	1.00 35.02
ATOM	2270	C	LEU	298				
					17.892	64.633	21.670	1.00 38.53
ATOM	2271	0	LEU	298	17.276	65.708	21.618	1.00 38.44
ATOM	2272	N	VAL	299	17.289	63.462	21.866	1.00 39.23
ATOM	2273	CA	VAL	299	15.839	63.389	22.054	1.00 40.08
MOTA	2274	CB	VAL	299	15.349	61.932	22.110	1.00 39.44
ATOM	2275	CG1	VAL	299	13.844	61.892	22.385	1.00 37.91
ATOM	2276	CG2	VAL	299	15.676	61.240	20.802	1.00 38.72
ATOM	2277	С	VAL	299	15.435	64.087	23.350	1.00 40.94
ATOM	2278	0	VAL	299	14.321	64.612	23.461	1.00 41.66
ATOM	2279	N	LEU	300	16.337	64.091	24.328	1.00 41.41
ATOM	2280	CA	LEU	300	16.043	64.737	25.600	1.00 42.31
ATOM	2281	CB	LEU	300	16.973	64.224	26.713	1.00 41.48
ATOM	2282	CG	LEU	300	16.943	62.766	27.206	1.00 40.38
ATOM	2283	CD1		300	17.677	62.711		1.00 40.14
ATOM	2284	CD2		300	15.517		28.545	
						62.251	27.380	1.00 38.74
MOTA	2285	С	LEU	300	16.204	66.251	25.444	1.00 43.44
ATOM	2286	0	LEU	300	15.304	67.020	25.806	1.00 43.84
ATOM	2287	N	LEU	301	17.346	66.675	24.898	1.00 43.90
ATOM	2288	CA	LEU	301	17.603	68.100	24.707	1.00 43.85
MOTA	2289	CB	LEU	301	18.895	68.335	23.919	1.00 43.20
ATOM	2290	CG	LEU	301	20.211	67.969	24.613	1.00 43.48
ATOM	2291		LEU	301	21.385	68.372	23.730	1.00 43.37
ATOM	2292	CD2		301	20.307	68.675	25.955	1.00 43.71
ATOM	2293	C	LEU	301	16.444	68.738	23.969	1.00 44.11
ATOM	2294	ō	LEU	301	16.068	69.875	24.254	1.00 44.38
ATOM	2294	N	ARG	302				1.00 44.35
					15.863	68.007	23.025	
MOTA	2296	CA	ARG	302	14.753	68.571	22.280	1.00 45.04

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ATOM	2297	CB	ARG	302	14.296	67.660	21.148	1.00 45.49
ATOM	2298	CG	ARG	302	13.082	68.256	20.468	1.00 45.91
ATOM	2299	CD	ARG	302	12.391	67.327	19.514	1.00 46.45
ATOM	2300	NE	ARG	302	11.194	67.985	19.007	1.00 47.37
ATOM	2301	CZ	ARG	302	10.423	67.503	18.043	1.00 48.12
ATOM	2302	NH1		302	10.719	66.344	17.466	1.00 48.80
				302	9.357	68.190	17.657	1.00 47.77
MOTA	2303	NH2	ARG					
MOTA	2304	C	ARG	302	13.577	68.807	23.196	1.00 45.13
MOTA	2305	0	ARG	302	12.982	69.885	23.198	1.00 45.57
ATOM	2306	N	LEU	303	13.228	67.787	23.966	1.00 45.14
MOTA	2307	CA	LEU	303	12.113	67.918	24.883	1.00 45.18
MOTA	2308	CB	LEU	303	11.952	66.624	25.695	1.00 44.02
MOTA	2309	CG	LEU	303	11.495	65.427	24.846	1.00 42.43
ATOM	2310		LEU	303	11.365	64.162	25.690	1.00 41.06
ATOM	2311		LEU	303	10.154	65.784	24.207	1.00 41.96
MOTA	2312	C	LEU	303	12.359	69.133	25.783	1.00 45.83
ATOM	2313	0	LEU	303	11.444	69.919	26.044	1.00 45.85
MOTA	2314	N	VAL	304	13.599	69.302	26.232	1.00 46.44
MOTA	2315	CA	VAL	304	13.943	70.440	27.085	1.00 47.76
ATOM	2316	CB	VAL	304	15.443	70.426	27.496	1.00 47.79
MOTA	2317	CG1	VAL	304	15.866	71.815	27.996	1.00 46.89
MOTA	2318	CG2	VAL	304	15.678	69.386	28.581	1.00 47.81
MOTA	2319	C	VAL	304	13.666	71.764	26.371	1.00 48.44
ATOM	2320	0	VAL	304	12.899	72.596	26.861	1.00 48.95
ATOM	2321	N	ASP	305	14.297	71.946	25.212	1.00 48.52
ATOM	2322	CA	ASP	305	14.143	73.165	24.432	1.00 48.31
ATOM	2323	CB	ASP	305	14.968	73.067	23.143	1.00 49.45
ATOM	2324	CG	ASP	305	16.441	72.715	23.412	1.00 51.00
ATOM	2325	OD1	ASP	305	17.056	73.323	24.317	1.00 50.99
ATOM	2326	OD2	ASP	305	16.994	71.834	22.715	1.00 51.84
ATOM	2327	C	ASP	305	12.677	73.460	24.122	1.00 47.77
ATOM	2328	o	ASP	305	12.341	74.541	23.641	1.00 48.22
ATOM	2329	N	GLU	306	11.799	72.505	24.407	1.00 46.84
ATOM	2330	CA	GLU	306	10.378	72.713	24.176	1.00 46.34
ATOM	2331	CB	GLU	306	9.831	71.683	23.184	1.00 46.20
ATOM	2332	CG	GLU	306	9.866	72.216	21.761	1.00 48.15
MOTA	2333	CD	GLU	306	9.571	71.175	20.692	1.00 49.26
ATOM	2334	OE1		306	8.514	70.499	20.768	1.00 50.03
ATOM	2335	OE2		306	10.398	71.049	19.759	1.00 49.62
ATOM	2336	C	GLU	306	9.635	72.661	25.493	1.00 45.99
ATOM	2337	ō	GLU	306	8.459	72.331	25.550	1.00 45.90
ATOM	2338	N	ASN	307	10.350	72.997	26.560	1.00 46.00
MOTA	2339	CA	ASN	307	9.787	73.029	27,902	1.00 45.60
ATOM	2340	CB	ASN	307	9.033	74.342	28.094	1.00 46.42
MOTA	2341	CG	ASN	307	9.971	75.531	28.224	1.00 46.98
ATOM	2342		ASN	307	10.435	75_849	29.321	1.00 47.63
ATOM	2343	ND2		307	10.273	76.181	27.102	1.00 46.93
ATOM	2344	C	ASN	307	8.886	71.853	28.246	1.00 45.05
ATOM	2345	ō	ASN	307	7.812	72.029	28.829	1.00 45.19
ATOM	2346	N	LEU	308	9.336	70.650	27.900	1.00 44.24
ATOM	2347	CA	LEU	308	8.575	69.439	28.180	1.00 43.28
ATOM	2348	CB	LEU	308	8.376	68.637	26.893	1.00 43.27
ATOM	2349	CG	LEU	308	7.070	68.825	26.115	1.00 44.09
ATOM	2350		LEU	308	6.765	70.294	25.935	1.00 44.22
ATOM	2351		LEU	308	7.182	68.139	24.760	1.00 43.94
ATOM	2351	CD	LEU	308	9.287	68.570	29.205	1.00 42.96
ATOM	2352	0	LEU	308	8.688	67.660	29.205	1.00 42.27
ATOM	2353	N	LEU	309	10.560	68.868	29.773	1.00 43.49
				309		68.077	30.371	1.00 44.85
MOTA	2355	CA	LEU	309	11.368	08.0//	30.3/1	1.00 44.00

Nummer: Offenlegungstag: 17. Juli 2003

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Figur 4

ATOM 2356 CB LEU 309 12.936 66.936 29.881 1.00 43.53 ATOM 2357 CD LEU 309 12.935 65.226 31.390 1.00 42.07 ATOM 2359 CD LEU 309 13.416 64.913 29.212 1.00 42.11 ATOM 2361 C LEU 309 13.416 64.913 29.212 1.00 42.11 ATOM 2361 C LEU 309 13.416 64.913 29.212 1.00 42.11 ATOM 2361 C LEU 309 13.074 69.777 30.518 1.00 46.01 ATOM 2361 C LEU 309 13.074 69.777 30.518 1.00 46.01 ATOM 2362 N PHE 310 12.625 68.601 32.397 1.00 47.92 ATOM 2363 CA PHE 310 13.608 69.293 33.238 1.00 49.25 ATOM 2364 CB PHE 310 13.608 69.293 33.238 1.00 49.25 ATOM 2365 CG PHE 310 15.013 69.093 32.666 1.00 46.24 ATOM 2365 CG PHE 310 15.013 69.093 32.666 1.00 46.04 ATOM 2365 CG PHE 310 15.043 67.650 32.590 1.00 47.06 ATOM 2365 CD PHE 310 15.438 67.650 32.590 1.00 47.06 ATOM 2365 CD PHE 310 15.438 67.650 32.590 1.00 46.63 ATOM 2366 CD1 PHE 310 14.947 66.715 33.497 1.00 46.63 ATOM 2369 CE2 PHE 310 15.344 65.385 33.433 1.00 45.27 ATOM 2370 CZ PHE 310 15.344 65.385 33.433 1.00 45.27 ATOM 2371 C PHE 310 15.244 65.385 33.433 1.00 45.27 ATOM 2371 C PHE 310 15.244 65.385 33.433 1.00 45.73 ATOM 2371 C PHE 310 13.292 70.785 33.145 1.00 51.16 ATOM 2377 CC PHE 310 14.185 71.616 33.561 1.00 55.80 ATOM 2373 N HIS 311 12.009 71.109 33.133 1.00 51.60 ATOM 2377 CG HIS 311 11.744 73.012 34.683 1.00 55.80 ATOM 2377 CG HIS 311 11.744 73.012 34.683 1.00 55.80 ATOM 2377 CD HIS 311 11.249 72.498 35.745 1.00 59.78 ATOM 2377 CD HIS 311 11.249 73.344 32.236 1.00 55.80 ATOM 2378 ND HIS 311 12.217 73.344 32.236 1.00 55.80 ATOM 2380 NE2 HIS 311 12.214 73.344 32.236 1.00 56.58 ATOM 2381 ND HIS 311 12.214 73.344 32.236 1.00 56.58 ATOM 2381 ND HIS 311 12.214 73.344 32.236 1.00 56.58 ATOM 2381 ND HIS 311 12.228 74.688 32.415 1.00 56.57 ATOM 2382 ND HIS 311 13.562 77.57 ATOM 2380 NE2 HIS 311 13.563 73.59 31.49 1.00 60.36 ATOM 2381 ND HIS 311 12.228 74.688 32.2461 1.00 56.56 ATOM 2382 ND HIS 311 12.288 74.688 32.2461 1.00 56.56 ATOM 2382 ND HIS 311 13.588 75.69 33.515 1.00 56.56 ATOM 2389 C GLU 313 15.586 77.09 34.246 35.250 1.00 56.56 ATOM 2389 C GLU 313 15.586 77.09 32.272 31.159 1.00		5ut -							
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ATOM 2367 CD2 PHE 310									
ATOM 2368 CRI PHE 310									
ATOM 2369 CE2 PHE 310									
ATOM 2370 CZ PHE 310	ATOM	2368	CE1		310	16.740	65.903	31.540	
ATOM 2371 C PHE 310 13.292 70.785 33.345 1.00 51.16 ATOM 2372 O PHE 310 14.185 71.616 33.561 1.00 50.84 ATOM 2373 N HIS 311 12.009 71.109 33.183 1.00 53.40 ATOM 2375 CB HIS 311 11.529 72.482 33.262 1.00 55.80 ATOM 2376 CB HIS 311 11.529 72.482 33.262 1.00 57.57 ATOM 2376 CG HIS 311 11.744 73.012 34.683 1.00 57.57 ATOM 2377 CD2 HIS 311 11.212 72.098 35.745 1.00 59.78 ATOM 2377 CD2 HIS 311 11.848 71.363 36.689 1.00 60.29 ATOM 2378 ND1 HIS 311 9.699 70.944 36.860 1.00 60.36 ATOM 2379 CE1 HIS 311 0.885 70.654 37.368 1.00 60.85 ATOM 2381 C HIS 311 12.214 73.384 32.236 1.00 56.24 ATOM 2382 O HIS 311 12.218 73.384 32.236 1.00 56.24 ATOM 2382 O HIS 311 12.218 73.384 32.236 1.00 56.87 ATOM 2383 N GUY 312 12.705 72.772 31.159 1.00 55.96 ATOM 2385 C GLY 312 14.820 73.522 30.109 1.00 55.96 ATOM 2385 C GLY 312 14.820 73.522 30.109 1.00 55.87 ATOM 2388 CA GLU 313 16.621 74.379 33.447 1.00 59.87 ATOM 2389 CB GLU 313 16.621 74.379 33.447 1.00 59.87 ATOM 2389 CB GLU 313 15.235 73.519 31.661 1.00 56.52 ATOM 2390 CG GLU 313 15.835 75.535 32.048 1.00 56.52 ATOM 2391 CG GLU 313 15.837 75.691 33.451 1.00 57.69 ATOM 2392 CD GLU 313 15.837 75.351 33.551 1.00 65.16 ATOM 2393 CB GLU 313 15.849 75.693 33.515 1.00 65.16 ATOM 2394 C GLU 313 15.849 75.693 33.515 1.00 65.60 6.24 ATOM 2395 C GLU 313 15.849 75.693 33.515 1.00 65.66 6.24 ATOM 2395 C GLU 313 15.849 75.693 33.515 1.00 65.66 6.24 ATOM 2395 C GLU 313 15.849 75.693 33.515 1.00 65.66 6.24 ATOM 2395 C GLU 313 15.849 75.693 33.515 1.00 65.66 6.24 ATOM 2395 C GLU 313 15.849 75.693 33.515 1.00 65.66 6.24 ATOM 2395 C GLU 313 15.849 75.693 33.515 1.00 65.66 6.24 ATOM 2395 C GLU 313 15.849 75.693 33.515 1.00 65.66 6.24 ATOM 2395 C GLU 313 15.849 75.693 33.515 1.00 65.66 6.24 ATOM 2395 C GLU 313 17.155 71.599 32.228 1.00 57.06 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 57.06 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 57.46 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400	MOTA	2369	CE2	PHE	310	15.344	65.385	33.433	1.00 46.27
ATOM 2372 O PHE 310 14.185 71.616 33.561 1.00 50.84 ATOM 2373 N HIS 311 12.009 71.109 33.262 1.00 55.80 ATOM 2376 CG HIS 311 11.529 72.482 33.262 1.00 55.80 ATOM 2376 CG HIS 311 11.212 72.098 35.745 1.00 59.78 ATOM 2376 CG HIS 311 11.212 72.098 35.745 1.00 59.78 ATOM 2377 CD2 HIS 311 11.212 72.098 35.745 1.00 59.78 ATOM 2377 CD2 HIS 311 11.848 71.363 36.689 1.00 60.29 ATOM 2378 ND1 HIS 311 9.697 71.815 35.879 1.00 60.36 ATOM 2379 CD2 HIS 311 11.848 71.363 36.689 1.00 60.29 ATOM 2379 CD2 HIS 311 10.885 70.664 37.368 1.00 60.85 ATOM 2380 NE2 HIS 311 0.885 70.664 37.368 1.00 66.85 ATOM 2380 NE2 HIS 311 12.212 73.384 32.236 1.00 56.24 ATOM 2380 C HIS 311 12.214 73.384 32.236 1.00 56.24 ATOM 2382 O HIS 311 12.214 73.384 32.236 1.00 56.24 ATOM 2382 O HIS 311 12.214 73.384 32.236 1.00 56.24 ATOM 2383 NG LY 312 12.288 74.608 32.415 1.00 55.87 ATOM 2385 C GLY 312 12.705 72.772 31.159 1.00 55.96 ATOM 2385 C GLY 312 12.705 72.772 31.159 1.00 55.96 ATOM 2385 C GLY 312 15.563 74.264 23.562 1.00 56.16 ATOM 2385 C GLY 312 15.563 74.264 23.562 1.00 56.58 ATOM 2385 C GLY 312 15.563 74.264 23.562 1.00 56.58 ATOM 2389 C GLU 313 16.621 73.765 32.048 1.00 57.69 ATOM 2389 C GLU 313 16.621 73.765 32.048 1.00 57.69 ATOM 2389 C GLU 313 16.621 73.765 32.048 1.00 57.69 ATOM 2389 C GLU 313 15.836 70.61 34.77 1.00 56.16 ATOM 2389 C GLU 313 15.836 70.61 34.72 1.00 56.56 ATOM 2399 C GLU 313 15.849 75.698 33.515 1.00 63.16 ATOM 2399 C GLU 313 15.849 75.698 33.515 1.00 65.16 ATOM 2399 C GLU 313 15.886 70.06 33.47 1.00 57.06 ATOM 2399 C GLU 313 15.886 70.06 33.497 1.00 56.64 ATOM 2399 C GLU 313 15.886 70.06 33.16 57.01 ATOM 2399 C GLU 313 17.439 72.484 32.011 1.00 57.06 ATOM 2399 C GLU 313 17.439 72.484 32.011 1.00 57.06 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.76 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.76 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.76 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.76 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.76 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.76 ATOM 2400 C SER 3	MOTA	2370	CZ	PHE	310	16.243	64.978	32.451	1.00 45.93
ATOM 2373 N HIS 311 12.009 71.109 33.183 1.00 53.40 ATOM 2374 CA HIS 311 11.529 72.482 33.262 1.00 55.80 ATOM 2375 CB HIS 311 11.744 73.012 34.683 1.00 57.57 ATOM 2376 CG HIS 311 11.212 72.098 35.745 1.00 59.78 ATOM 2377 CD2 HIS 311 11.848 71.363 36.689 1.00 60.29 ATOM 2378 ND1 HIS 311 9.697 71.815 35.899 1.00 60.36 ATOM 2379 CE1 HIS 311 9.697 70.644 36.660 1.00 60.99 ATOM 2380 NEZ HIS 311 10.885 70.654 37.368 1.00 60.85 ATOM 2381 C HIS 311 12.214 73.384 32.236 1.00 56.24 ATOM 2382 O HIS 311 12.214 73.384 32.236 1.00 56.24 ATOM 2382 O HIS 311 12.288 74.608 32.415 1.00 56.87 ATOM 2383 N GUY 312 12.705 72.772 31.159 1.00 55.96 ATOM 2385 C GUY 312 14.820 73.804 30.402 1.00 56.87 ATOM 2386 C GUY 312 15.563 74.264 29.552 1.00 56.16 ATOM 2387 N GUI 313 16.521 73.756 32.048 1.00 57.69 ATOM 2388 CA GLU 313 16.521 73.756 32.048 1.00 57.69 ATOM 2390 CG GLU 313 16.521 73.756 32.048 1.00 57.69 ATOM 2391 CD GUU 313 15.889 75.698 33.515 1.00 65.16 ATOM 2392 CD GUU 313 15.889 75.698 33.515 1.00 65.16 ATOM 2392 CD GUU 313 15.889 75.698 33.515 1.00 65.16 ATOM 2393 C G GLU 313 15.889 75.698 33.515 1.00 65.16 ATOM 2394 C GLU 313 15.889 75.698 33.515 1.00 65.16 ATOM 2392 CD GUU 313 15.889 75.698 33.515 1.00 65.16 ATOM 2393 C G GLU 313 15.889 75.698 33.515 1.00 65.16 ATOM 2394 C GLU 313 15.889 75.698 33.515 1.00 65.16 ATOM 2393 CD GLU 313 15.889 75.698 33.515 1.00 65.16 ATOM 2394 C GLU 313 15.889 75.698 33.515 1.00 65.16 ATOM 2395 C GUU 313 15.889 75.698 33.515 1.00 65.66 ATOM 2397 CA ALA 314 19.316 71.305 31.029 1.00 56.67 ATOM 2398 C G GLU 313 17.439 72.484 32.011 1.00 57.06 ATOM 2399 C ALA 314 19.316 71.305 31.029 1.00 56.76 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2401 C G GLU 316 22.477 71.774 32.580 1.00 56.75 ATOM 2402 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2409 C SEU 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00	ATOM	2371	С	PHE	310	13.292	70.785	33.345	1.00 51.16
ATOM 2374 CA HIS 311 11.529 72.482 32.262 1.00 55.80 ATOM 2375 CB HIS 311 11.744 73.012 34.683 1.00 57.57 ATOM 2376 CG HIS 311 11.212 72.098 35.745 1.00 59.78 ATOM 2377 CD2 HIS 311 11.848 71.363 36.689 1.00 60.29 ATOM 2379 CE1 HIS 311 9.699 70.944 36.860 1.00 60.99 ATOM 2381 C HIS 311 10.885 70.654 37.368 1.00 60.85 ATOM 2381 C HIS 311 12.214 73.384 32.236 1.00 56.24 ATOM 2383 N GU 312 12.705 72.772 31.159 1.00 55.96 ATOM 2385 C GLY 312 <td>MOTA</td> <td>2372</td> <td>0</td> <td>PHE</td> <td>310</td> <td>14.185</td> <td>71.616</td> <td>33.561</td> <td>1.00 50.84</td>	MOTA	2372	0	PHE	310	14.185	71.616	33.561	1.00 50.84
ATOM 2375 CB HIS 311 11.714 73.012 34.883 1.00 57.57 ATOM 2376 CG HIS 311 11.212 72.098 35.745 1.00 59.78 ATOM 2377 CD2 HIS 311 11.818 71.363 36.899 1.00 60.29 ATOM 2378 ND1 HIS 311 9.867 71.815 35.879 1.00 60.36 ATOM 2379 CEI HIS 311 9.867 70.944 36.860 1.00 60.39 ATOM 2380 ND HIS 311 10.885 70.654 37.368 1.00 60.85 ATOM 2381 C HIS 311 12.218 73.384 32.236 1.00 56.24 ATOM 2382 O HIS 311 12.218 73.384 32.236 1.00 56.24 ATOM 2382 O HIS 311 12.218 74.608 32.415 1.00 55.87 ATOM 2382 O HIS 311 12.288 74.608 32.415 1.00 55.87 ATOM 2385 C GLY 312 12.705 72.772 31.159 1.00 55.96 ATOM 2385 C GLY 312 13.366 73.522 30.109 1.00 55.87 ATOM 2385 C GLY 312 15.563 74.264 29.552 1.00 56.16 ATOM 2389 C GLU 313 15.235 73.599 31.666 1.00 56.58 ATOM 2387 N GLU 313 15.235 73.599 31.666 1.00 57.69 ATOM 2389 CG GLU 313 16.521 73.755 32.048 1.00 57.69 ATOM 2389 CG GLU 313 16.521 73.756 32.048 1.00 57.69 ATOM 2390 CG GLU 313 15.886 75.698 33.515 1.00 66.12 ATOM 2391 CD GLU 313 15.886 75.698 33.515 1.00 66.31 ATOM 2392 CG GLU 313 15.886 75.698 33.515 1.00 66.31 ATOM 2393 CC GLU 313 15.886 75.698 33.515 1.00 66.31 ATOM 2393 CC GLU 313 15.886 77.096 35.457 1.00 66.31 ATOM 2393 CC GLU 313 15.886 77.096 35.595 1.00 66.01 ATOM 2393 CC GLU 313 15.886 77.096 35.595 1.00 66.01 ATOM 2393 CC GLU 313 15.886 77.096 35.550 1.00 66.01 ATOM 2393 CC GLU 313 17.359 72.484 32.011 1.00 67.06 ATOM 2397 CA ALA 314 19.316 71.305 31.029 1.00 66.01 ATOM 2398 C ALA 314 19.316 71.305 31.029 1.00 66.05 ATOM 2398 C ALA 314 19.316 71.305 31.029 1.00 56.67 ATOM 2398 C ALA 314 19.316 71.305 31.029 1.00 56.76 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 57.06 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.75 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.75 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.75 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.15	ATOM	2373	N	HIS	311	12.009	71.109	33.183	1.00 53.40
ATOM 2376 CG HIS 311 11.848 71.363 36.89 1.00 59.78 ATOM 2377 CD2 HIS 311 9.867 71.815 35.879 1.00 60.29 ATOM 2378 ND1 HIS 311 9.867 71.815 35.879 1.00 60.39 ATOM 2379 CE1 HIS 311 9.897 70.944 36.890 1.00 60.39 ATOM 2381 C HIS 311 10.885 70.654 37.368 1.00 60.89 ATOM 2381 C HIS 311 12.214 73.384 32.236 1.00 56.24 ATOM 2381 C HIS 311 12.214 73.384 32.236 1.00 56.24 ATOM 2382 C HIS 311 12.288 74.608 32.415 1.00 56.87 ATOM 2384 CA GLY 312 12.705 72.772 31.159 1.00 55.96 ATOM 2385 C GLY 312 13.366 73.522 30.109 1.00 55.87 ATOM 2385 C GLY 312 15.563 74.254 23.552 1.00 56.18 ATOM 2385 C GLY 312 15.563 74.254 23.552 1.00 56.58 ATOM 2385 C GLY 312 15.563 74.254 23.552 1.00 56.58 ATOM 2385 C GLY 312 15.563 74.254 23.552 1.00 56.58 ATOM 2385 C GLY 312 15.563 74.254 23.552 1.00 56.58 ATOM 2385 C GLY 312 15.563 74.554 20.48 1.00 56.55 ATOM 2389 CB GLU 313 15.235 73.519 31.646 1.00 56.55 ATOM 2389 CB GLU 313 16.612 74.379 33.447 1.00 59.84 ATOM 2390 CC GLU 313 15.849 75.698 33.155 1.00 65.16 ATOM 2391 C GLU 313 15.849 75.698 33.155 1.00 65.16 ATOM 2392 C GLU 313 15.849 75.698 33.155 1.00 65.16 ATOM 2393 CC GLU 313 15.849 75.698 33.155 1.00 66.01 ATOM 2393 C GLU 313 15.849 75.698 33.155 1.00 65.16 ATOM 2393 C GLU 313 15.849 75.698 33.155 1.00 66.01 ATOM 2393 C GLU 313 15.849 75.698 33.155 1.00 65.16 ATOM 2393 C GLU 313 15.849 75.09 35.455 1.00 66.01 ATOM 2393 C GLU 313 15.849 75.09 35.455 1.00 66.01 ATOM 2393 C GLU 313 15.849 75.09 35.455 1.00 66.01 ATOM 2393 C GLU 313 15.849 75.253 32.228 1.00 57.06 ATOM 2398 C GLU 313 17.155 71.529 32.728 1.00 57.06 ATOM 2398 C GLU 313 17.155 71.529 32.728 1.00 57.06 ATOM 2400 C ALA 314 19.316 71.305 31.029 1.00 56.56 ATOM 2402 C G SER 315 22.666 69.029 33.624 1.00 55.42 ATOM 2402 C G SER 315 22.891 68.868 34.130 1.00 55.42 ATOM 2403 C G GLU 316 23.693 70.463 34.757 1.00 55.45 ATOM 2403 C G GLU 316 23.895 70.416 30.793 1.00 55.45 ATOM 2403 C G GLU 316 23.693 70.464 33.400 C GLU 316 23.693 70.463 34.130 1.00 55.42 ATOM 2403 C G GLU 316 23.693 70.463 34.130 1.00 55.42 ATOM 2403 C G GLU 316 2	MOTA	2374	CA	HIS	311	11.529	72.482	33.262	1.00 55.80
ATOM 2377 CD2 HIS 311 11.848 71.363 36.889 1.00 60.29 ATOM 2378 ND1 HIS 311 9.867 71.815 35.879 1.00 60.36 ATOM 2379 CEI HIS 311 9.869 70.944 36.860 1.00 60.36 ATOM 2380 NE2 HIS 311 12.214 73.384 32.236 1.00 56.24 ATOM 2382 O HIS 311 12.214 73.384 32.236 1.00 56.24 ATOM 2382 O HIS 311 12.214 73.384 32.236 1.00 56.87 ATOM 2385 C GLY 312 12.705 72.772 31.159 1.00 55.96 ATOM 2385 C GLY 312 14.820 73.522 30.109 1.00 55.96 ATOM 2385 C GLY 312 13.366 73.522 30.109 1.00 55.96 ATOM 2385 C GLY 312 15.563 74.264 29.562 1.00 56.16 ATOM 2385 C GLY 312 15.563 74.264 29.562 1.00 56.58 ATOM 2387 N GLU 313 15.235 73.519 31.664 1.00 57.69 ATOM 2389 CB GLU 313 16.521 73.755 32.048 1.00 57.69 ATOM 2389 CB GLU 313 16.521 73.755 32.048 1.00 57.69 ATOM 2390 CG GLU 313 15.838 76.691 34.74 1.00 59.84 ATOM 2391 CD GLU 313 15.838 76.601 34.95 1.00 65.16 ATOM 2392 CD GLU 313 15.838 76.061 34.955 1.00 65.16 ATOM 2392 CD GLU 313 15.538 75.698 33.515 1.00 65.16 ATOM 2392 CD GLU 313 15.538 76.061 34.955 1.00 65.16 ATOM 2392 CD GLU 313 15.888 70.601 34.955 1.00 65.16 ATOM 2392 CD GLU 313 15.538 76.061 34.955 1.00 65.16 ATOM 2392 CD GLU 313 15.538 76.061 34.955 1.00 65.16 ATOM 2392 CD GLU 313 17.359 71.693 35.557 1.00 65.16 ATOM 2392 CD GLU 313 17.359 71.593 31.505 1.00 65.16 ATOM 2392 CD GLU 313 17.359 71.593 32.728 1.00 65.01 ATOM 2393 CD GLU 313 17.359 71.593 32.728 1.00 65.01 ATOM 2393 CD GLU 313 17.359 71.593 32.728 1.00 65.01 ATOM 2398 CA ALA 314 19.316 71.305 31.029 1.00 65.634 ATOM 2398 CB ALA 314 19.316 71.305 31.029 1.00 56.647 ATOM 2398 CB ALA 314 19.316 71.305 31.029 1.00 56.65 ATOM 2398 CB ALA 314 19.316 71.305 31.029 1.00 56.76 ATOM 2400 CB SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 CB SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 CB SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 CB SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 CB SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 CB SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 CB SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 CB SER 315 22.666 69.029 33.	MOTA	2375	CB	HIS	311	11.744			1.00 57.57
ATOM 2377 CD2 HIS 311 11.848 71.363 36.899 1.00 60.29 ATOM 2378 ND1 HIS 311 9.697 70.944 36.860 1.00 60.36 ATOM 2379 CEI HIS 311 9.699 70.944 36.860 1.00 60.36 ATOM 2300 NEZ HIS 311 10.885 70.944 36.860 1.00 60.36 ATOM 2381 C HIS 311 12.214 73.384 32.236 1.00 56.87 ATOM 2381 C HIS 311 12.214 73.384 32.236 1.00 56.87 ATOM 2383 N GLY 312 12.705 72.772 31.159 1.00 56.87 ATOM 2385 C GLY 312 12.705 73.522 30.109 1.00 55.96 ATOM 2385 C GLY 312 14.820 73.804 30.402 1.00 56.16 ATOM 2385 C GLY 312 15.563 74.264 29.552 1.00 56.58 ATOM 2387 N GLU 313 15.235 73.519 31.664 1.00 56.58 ATOM 2387 N GLU 313 15.235 73.519 31.664 1.00 56.52 ATOM 2389 CB GLU 313 16.521 73.755 32.048 1.00 57.69 ATOM 2389 CB GLU 313 16.521 73.755 32.048 1.00 57.69 ATOM 2390 CG GLU 313 15.889 75.698 33.515 1.00 63.16 ATOM 2391 CD GLU 313 15.889 75.698 33.515 1.00 63.16 ATOM 2392 CD GLU 313 15.588 76.061 34.925 1.00 65.16 ATOM 2392 CD GLU 313 15.588 76.061 34.925 1.00 65.16 ATOM 2392 CD GLU 313 15.588 70.061 34.925 1.00 65.16 ATOM 2395 C GLU 313 15.888 77.095 35.455 1.00 65.16 ATOM 2395 C GLU 313 15.588 70.061 34.925 1.00 65.16 ATOM 2395 C GLU 313 15.588 70.061 34.925 1.00 65.16 ATOM 2395 C GLU 313 15.888 70.601 34.925 1.00 65.16 ATOM 2395 C GLU 313 17.155 71.529 32.728 100 57.09 ATOM 2395 C GLU 313 17.155 71.529 32.728 100 57.06 ATOM 2395 C GLU 313 17.155 71.529 32.728 100 57.06 ATOM 2395 C GLU 313 17.155 71.529 32.728 100 57.06 ATOM 2395 C GLU 313 17.155 71.529 32.728 100 57.06 ATOM 2395 C GLU 313 17.155 71.529 32.728 100 57.06 ATOM 2400 C ALA 314 19.316 71.305 31.029 1.00 56.56 ATOM 2397 C ALA 314 19.316 71.305 31.029 1.00 56.76 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 57.46 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 57.46 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.73 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.56 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.54 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.56 ATOM 2400 C SER 315 22.666 69.029 33.624 1.00 56.56 ATOM 2400 C	MOTA	2376	CG	HIS	311	11.212	72.098	35.745	1.00 59.78
ATOM 2378 ND1 HIS 311 9.867 71.815 35.879 1.00 60.36 ATOM 2379 CE1 HIS 311 10.885 70.654 37.368 1.00 60.99 ATOM 2380 NE2 HIS 311 10.885 70.654 37.368 1.00 60.85 ATOM 2381 C HIS 311 12.214 73.384 32.226 1.00 56.24 ATOM 2382 O HIS 311 12.288 74.608 32.415 1.00 55.87 ATOM 2383 N GLY 312 12.705 72.772 31.159 1.00 55.87 ATOM 2385 C GLY 312 13.366 73.522 30.109 1.00 55.87 ATOM 2386 C GLY 312 13.366 73.522 30.109 1.00 55.86 ATOM 2386 N GLY 312 15.563 74.264 23.552 1.00 56.58 ATOM 2387 N GLU 313 15.235 73.519 31.646 1.00 56.58 ATOM 2388 C G GLY 312 15.563 74.264 23.552 1.00 56.58 ATOM 2388 C G GLY 312 15.563 73.519 31.646 1.00 56.58 ATOM 2389 C G GLU 313 16.612 74.379 33.447 1.00 59.84 ATOM 2389 C G GLU 313 15.849 75.698 33.515 1.00 65.16 ATOM 2391 C G GLU 313 15.849 75.698 33.515 1.00 65.16 ATOM 2392 OEI GLU 313 15.849 75.698 33.515 1.00 65.16 ATOM 2393 OZ GLU 313 15.858 77.096 35.455 1.00 66.01 ATOM 2393 OZ GLU 313 15.858 77.096 35.455 1.00 66.01 ATOM 2395 C G GLU 313 15.858 77.096 35.455 1.00 66.01 ATOM 2395 C G GLU 313 15.858 77.096 35.455 1.00 66.01 ATOM 2395 C G GLU 313 15.858 77.096 35.455 1.00 66.01 ATOM 2395 C G GLU 313 15.858 77.096 35.455 1.00 66.34 ATOM 2395 C G GLU 313 15.858 77.096 35.455 1.00 66.01 ATOM 2395 C G GLU 313 15.858 77.096 35.455 1.00 66.01 ATOM 2395 C G GLU 313 17.439 72.484 32.011 1.00 57.06 ATOM 2395 C G ALA 314 19.316 71.305 31.029 1.00 56.56 ATOM 2398 C B ALA 314 19.316 71.305 31.029 1.00 56.56 ATOM 2399 C ALA 314 20.599 71.490 31.643 1.00 56.94 ATOM 2400 C ALA 314 20.599 71.490 31.643 1.00 56.94 ATOM 2401 N SER 315 22.666 69.029 33.624 1.00 57.46 ATOM 2402 C S SER 315 22.666 69.029 33.624 1.00 57.39 ATOM 2405 C SER 315 23.895 68.868 34.10 1.00 57.39 ATOM 2406 C SER 315 23.895 68.868 34.10 1.00 57.39 ATOM 2407 C G GLU 316 28.487 73.343 31.466 1.00 63.44 ATOM 2410 C G GLU 316 28.487 73.343 31.466 1.00 63.44 ATOM 2410 C G GLU 316 28.487 73.343 31.466 1.00 63.46 ATOM 2410 C G GLU 316 28.487 73.343 31.466 1.00 63.46	ATOM	2377	CD2	HIS	311				
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ATOM 2405 C SER 315 23.673 70.627 32.003 1.00 55.00 ATOM 2407 N GLU 316 22.595 70.416 30.793 1.00 55.42 ATOM 2407 N GLU 316 24.776 71.070 32.598 1.00 55.42 ATOM 2408 CA GLU 316 26.012 71.346 31.875 1.00 57.46 ATOM 2410 CG GLU 316 27.111 71.754 32.860 1.00 58.71 ATOM 2410 CG GLU 316 22.458 72.050 32.206 1.00 60.34 ATOM 2411 CD GLU 316 28.482 73.343 31.406 1.00 61.64 ATOM 2412 OE1 GLU 316 28.288 74.420 32.031 1.00 62.41 ATOM 2413 OE2 GLU 316 28.288 74.420 32.031 1.00 62.41 ATOM 2413 OE2 GLU 316 28.587 47.3280 30.160 1.00 61.76									
ATOM 2406 O SER 315 23.595 70.416 30.793 1.00 55.42 ATOM 2407 N GLU 316 24.776 71.070 32.598 1.00 55.42 ATOM 2408 CA GLU 316 26.012 71.346 31.875 1.00 57.46 ATOM 2409 CB GLU 316 27.111 71.754 32.860 1.00 58.71 ATOM 2410 CG GLU 316 28.458 72.050 32.206 1.00 60.34 ATOM 2411 CD' GLU 316 28.458 72.050 32.206 1.00 60.34 ATOM 2412 OE1 GLU 316 28.288 74.420 32.031 1.00 61.66 ATOM 2413 OE2 GLU 316 28.288 74.420 32.031 1.00 62.41 ATOM 2413 OE2 GLU 316 28.288 74.420 32.031 1.00 62.41 ATOM 2413 OE2 GLU 316 28.574 73.280 30.160 1.00 61.76									
ATOM 2407 N GLU 316 24.776 71.070 32.558 1.00 56.67 ACM 2408 CA GLU 316 26.012 71.346 31.875 1.00 57.46 ATOM 2409 CB GLU 316 27.111 71.754 32.860 1.00 58.71 ATOM 2410 CG GLU 316 28.458 72.050 32.206 1.00 58.71 ATOM 2411 CD GLU 316 28.452 73.343 31.406 1.00 61.64 ATOM 2412 021 GLU 316 28.288 74.420 32.031 1.00 62.41 ATOM 2413 022 GLU 316 28.574 73.280 30.160 1.00 61.76									
ATOM 2408 CA GLU 316 26,012 71.346 31.875 1.00 57.46 ATOM 2409 CB GLU 316 27.111 71.754 32.860 1.00 58.71 ATOM 2410 CG GLU 316 28.458 72.050 32.206 1.00 60.34 ATOM 2411 CD' GLU 316 28.442 73.343 31.406 1.00 61.64 ATOM 2412 OE1 GLU 316 28.288 74.420 32.031 1.00 62.41 ATOM 2413 OE2 GLU 316 28.574 73.280 30.160 1.00 61.76									
ATOM 2409 C8 GLU 316 27.111 71.754 32.860 1.00 58.71 ATOM 2410 CG GLU 316 28.458 72.050 32.206 1.00 60.34 ATOM 2411 CD GLU 316 28.442 73.343 31.406 1.00 61.64 ATOM 2412 O21 GLU 316 28.288 74.420 32.031 1.00 62.41 ATOM 2413 OE2 GLU 316 28.574 73.280 30.160 1.00 61.76									
ATOM 2410 CG GLU 316 28.458 72.050 32.206 1.00 60.34 ATOM 2411 CD GLU 316 28.442 73.343 31.406 1.00 61.64 ATOM 2412 021 GLU 316 28.288 74.420 32.031 1.00 62.41 ATOM 2413 0E2 GLU 316 28.574 73.280 30.160 1.00 61.76									
ATOM 2411 CD: GLU 316 28.442 73.343 31.406 1.00 61.64 ATOM 2412 0E1 GLU 316 28.288 74.420 32.031 1.00 62.41 ATOM 2413 0E2 GLU 316 28.574 73.280 30.160 1.00 61.76									
ATOM 2412 OE1 GLU 316 28.288 74.420 32.031 1.00 62.41 ATOM 2413 OE2 GLU 316 28.574 73.280 30.160 1.00 61.76									
ATOM 2413 OE2 GLU 316 28.574 73.280 30.160 1.00 61.76									
ATOM 2414 C GLU 316 26.442 70.078 31.161 1.00 57.35									
	ATOM	2414	C	GLU	316	25.442	70.078	31.161	1.00 57.35

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Figur 4

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ATOM	2415	0	GLU	316	26.770	70.088	20 072	1 00 57 68
ATOM	2415	N	GLN	317			29.972	1.00 57.68
					26.439	68.988	31.920	1.00 56.84
ATOM	2417	CA	GLN	317	26.817	67.677	31.427	1.00 56.23
ATOM	2418	CB	GLN	317	26.760	66.669	32.580	1.00 55.93
MOTA	2419	CG	GLN	317	27.504	67.113	33.840	1.00 55.46
ATOM	2420	CD	GLN	317	27.063	66.355	35.085	1.00 55.01
MOTA	2421	OE1	GLN	317	27.246	65.140	35.194	1.00 54.83
MOTA	2422	NE2		317	26.468	67.074	36.029	1.00 54.68
MOTA	2423	C	GLN	317	25.902	67.210	30.290	1.00 56.37
MOTA	2424	0	GLN	317	26.376	66.634	29.312	1.00 56.16
ATOM	2425	N	LEU	318	24.599	67.476	30.412	1.00 56.41
MOTA	2426	CA	LEU	318	23.616	67.043	29.413	1.00 56.48
MOTA	2427	CB	LEU	318	22.190	67.333	29.890	1.00 55.59
MOTA	2428	CG	LEU	318	21.084	66.700	29.034	1.00 54.71
MOTA	2429	CD1	LEU	318	21.090	65.191	29.231	1.00 53.88
ATOM	2430	CD2	LEU	318	19.731	67.268	29.422	1.00 54.28
ATOM	2431	C	LEU	318	23.784	67.621	28.017	1.00 56.99
ATOM	2432	0	LEU	318	23.692	66.893	27.029	1.00 57.21
MOTA	2433	N	ARG	319	24.011	68.924	27.919	1.00 57.16
MOTA	2434	CA	ARG	319	24.177	69.530	26.606	1.00 57.68
ATOM	2435	CB	ARG	319	23.870	71.026	26.690	1.00 59.32
MOTA	2436	CG	ARG	319	22.420	71.284	27.105	1.00 62.20
ATOM	2437	CD	ARG	319	22.125	72.743	27.401	1.00 64.53
MOTA	2438	NE	ARG	319	20.758	72.927	27.892	1.00 66.89
MOTA	2439	CZ	ARG	319	20.297	74.055	28.433	1.00 68.29
ATOM	2440	NH1	ARG	319	21.096	75.112	28.555	1.00 68.30
ATOM	2441		ARG	319	19.034	74.127	28.851	1.00 68.25
ATOM	2442	C	ARG	319	25.587	69.278	26.081	1.00 57.09
ATOM	2443	ō	ARG	319	26.049	69.951	25.160	1.00 57.05
ATOM	2444	N	THR	320	26.246	68.277	26.667	1.00 56.25
ATOM	2445	CA	THR	320	27.612	67.888	26.318	1.00 55.15
ATOM	2446	CB	THR	320	28.478	67.836	27.589	1.00 54.85
ATOM	2447		THR	320	28.601	69.158	28.133	1.00 54.94
ATOM	2448	CG2	THR	320	29.854	67.262	27.287	1.00 54.63
ATOM	2449	C	THR	320	27.689	66.524	25.613	1.00 55.04
ATOM	2450	ō	THR	320	27.476	65.480	26.229	1.00 55.13
ATOM	2451	N	ARG	321	28.017	66.536	24.326	1.00 54.38
ATOM	2452	CA	ÀRG	321	28.106	65.304	23.545	1.00 54.36
ATOM	2453	CB	ARG	321	28.841	65.586	22.236	1.00 56.05
ATOM	2454	CG	ARG	321	28.153	66.651	21.402	1.00 59.03
ATOM	2455	CD	ARG	321	28.943	67.013	20.156	1.00 61.60
ATOM	2456	NE	ARG	321	28.331	68.123	19.426	1.00 63.68
ATOM	2457	CZ	ARG	321	28.909	68.753	18.406	1.00 65.43
ATOM	2458	NH1		321	30.119	68.381	17.997	1.00 65.83
ATOM	2459	NH2	ARG	321	28.280	69.750	17.792	1.00 65.76
ATOM	2460	C	ARG	321	28.765	64 .123	24.262	1.00 52.97
MOTA	2461	ō	ARG	321	29.885	64.234	24.758	1.00 53.13
MOTA	2462	N	GLY	322	28.056	62.996	24.316	1.00 51.39
ATOM	2463	CA	GLY	322	28.592	61.802	24.950	1.00 49.22
ATOM	2464	c	GLY	322	28.198	61.609	26.402	1.00 48.17
ATOM	2465	ō	GLY	322	28.450	60.550	26.986	1.00 48.17
ATOM	2466	N	ALA	323	27.574	62.627	26.988	1.00 46.66
ATOM	2467	CA	ALA	323	27.150	62.573	28.385	1.00 44.99
ATOM	2468	CB	ALA	323	26.462	63.861	28.761	1.00 45.87
ATOM	2469	C	ALA	323	26.224	61.403	28.676	1.00 43.43
ATOM	2470	ō	ALA	323	26.514	60.562	29.530	1.00 43.43
ATOM	2471	N	PHE	324	25.094	61.361	27.981	1.00 41.61
ATOM	2472	CA	PHE	324	24.147	60.282	28.185	1.00 40.44
ATOM	2473	CB	PHE	324	22.797	60.631	27.564	1.00 38.94
111011	2413		2112	324	22.191	30.031	21.504	1.00 30.34

Figur 4

NTOM		-							
ATOM	ATOM	2474	CG	PHE	324	21 644	50 998	28 262	1 00 38 08
ATOM 2476 CD2 PHE 324 20.105 58.733 27.860 1.00 36.96 ATOM 2477 CE1 PHE 324 20.010 59.998 30.050 1.00 37.79 ATOM 2478 CZ2 PHE 324 20.116 58.105 28.542 1.00 37.79 ATOM 2479 CZ PHE 324 19.555 58.739 29.643 1.00 37.79 ATOM 2480 C PHE 324 24.721 59.033 27.525 1.00 40.11 ATOM 2481 C PHE 324 24.721 59.033 27.525 1.00 40.11 ATOM 2481 C PHE 324 24.721 59.033 27.525 1.00 40.11 ATOM 2482 N GUJ 325 25.129 58.072 28.350 1.00 39.06 ATOM 2483 C G GUJ 325 25.129 58.072 28.350 1.00 39.06 ATOM 2484 C G GUJ 325 25.129 56.681 27.841 1.00 37.85 ATOM 2484 C G GUJ 325 26.846 56.418 28.781 1.00 38.17 ATOM 2485 C G GUJ 325 27.790 57.528 29.085 1.00 40.68 ATOM 2487 ORI GUJ 325 28.653 56.608 31.086 1.00 44.06 ATOM 2489 C G GUJ 325 28.653 56.608 31.086 1.00 44.06 ATOM 2489 C G GUJ 325 28.653 56.608 31.086 1.00 44.06 ATOM 2489 C G GUJ 325 24.799 55.693 27.641 1.00 36.60 ATOM 2490 C GUJ 325 22.903 57.481 29.90 1.00 44.51 ATOM 2491 N THR 326 25.903 57.452 28.477 1.00 37.31 ATOM 2492 C A THR 326 25.193 53.455 28.47 1.00 35.30 ATOM 2493 CB THR 326 24.875 52.921 25.207 1.00 31.58 ATOM 2494 C C THR 326 24.875 52.921 25.207 1.00 31.58 ATOM 2495 C C THR 326 24.875 52.921 25.207 1.00 31.58 ATOM 2497 C THR 326 24.934 53.617 23.956 1.00 29.82 ATOM 2498 C C THR 326 24.935 53.016 27.515 1.00 33.05 ATOM 2497 C THR 326 22.846 52.588 27.742 1.00 33.05 ATOM 2498 C C THR 326 24.935 53.016 27.515 1.00 33.05 ATOM 2498 C C THR 326 23.951 53.016 27.515 1.00 33.05 ATOM 2498 C C THR 326 24.935 53.016 27.515 1.00 33.05 ATOM 2498 C C THR 326 24.935 53.016 27.515 1.00 33.05 ATOM 2498 C C THR 326 23.951 53.016 27.515 1.00 33.05 ATOM 2499 C C A RG 327 24.859 52.882 39.49 1.00 32.29 ATOM 2490 C G ARG 327 26.146 52.245 30.417 1.00 38.88 ATOM 2500 C B ARG 327 27.956 51.063 32.97 1.00 38.88 ATOM 2501 C C ARG 327 26.146 52.245 30.417 1.00 38.89 ATOM 2501 C C ARG 327 27.956 51.063 30.940 1.00 29.96 ATOM 2501 C C ARG 327 28.815 53.070 30.940 1.00 29.95 ATOM 2501 C C ARG 327 28.815 53.070 30.940 1.00 29.95 ATOM 2501 C C ARG 327 28.815 53.050 30.940 1.00 29.95 ATOM 2510 C C A									
ATOM 2477 CE1 PHE 324 20.110 59.998 30.050 1.00 37.11 ATOM 2478 CE2 PHE 324 19.555 58.739 29.643 1.00 37.73 ATOM 2480 C PHE 324 19.555 58.739 29.643 1.00 37.73 ATOM 2480 C PHE 324 24.721 59.033 27.525 1.00 40.11 ATOM 2481 O PHE 324 24.721 59.033 27.525 1.00 40.11 ATOM 2482 N GUU 325 25.129 58.072 28.550 1.00 39.06 ATOM 2482 N GUU 325 25.740 56.851 27.844 1.00 37.85 ATOM 2482 C G GUU 325 27.790 57.528 29.055 1.00 40.68 ATOM 2485 C G GUU 325 27.990 57.528 29.055 1.00 40.68 ATOM 2487 O D GUU 325 28.653 56.083 1.00 39.06 ATOM 2487 O D GUU 325 28.653 56.083 1.00 38.17 ATOM 2487 O D GUU 325 28.653 56.083 1.00 38.17 ATOM 2487 O D GUU 325 28.653 56.083 1.00 38.17 ATOM 2489 C GUU 325 28.922 57.075 29.951 1.00 42.47 ATOM 2489 C GUU 325 24.799 55.693 27.641 1.00 36.60 ATOM 2491 N THR 326 24.799 55.693 27.641 1.00 37.31 ATOM 2492 C A THR 326 24.193 53.816 26.245 1.00 33.37 ATOM 2493 C GUU 325 23.903 55.445 28.447 1.00 37.31 ATOM 2493 C GUU 325 24.999 53.816 26.245 1.00 33.37 ATOM 2493 C GUU 325 24.999 53.816 26.245 1.00 33.37 ATOM 2493 C GUU 325 24.999 53.816 26.245 1.00 33.37 ATOM 2493 C GUU 325 23.903 55.445 28.447 1.00 37.31 ATOM 2493 C GU THR 326 24.975 56.693 27.641 1.00 36.60 ATOM 2493 C GU THR 326 24.975 56.693 27.641 1.00 37.31 ATOM 2493 C GU THR 326 24.875 52.921 25.707 1.00 31.58 ATOM 2493 C GU THR 326 24.875 52.921 25.707 1.00 31.58 ATOM 2493 C GU THR 326 24.875 52.921 25.707 1.00 31.58 ATOM 2493 C GU THR 326 24.875 52.921 25.707 1.00 31.58 ATOM 2499 C GU THR 326 22.846 52.292 27.707 30.80 31.58 ATOM 2499 C GU THR 326 22.846 52.292 27.707 30.80 31.58 ATOM 2499 C GU THR 326 23.935 51.00 33.07 7.00 33.05 ATOM 2499 C GU THR 326 23.935 51.00 33.07 7.00 33.05 ATOM 2499 C GU THR 326 23.935 51.00 33.07 7.00 33.05 ATOM 2499 C GU THR 326 23.935 51.00 33.07 7.00 33.05 ATOM 2499 C GU THR 326 23.935 51.00 33.07 7.00 33.05 ATOM 2500 C GU THR 326 23.935 51.00 33.07 7.00 33.05 ATOM 2500 C GU THR 326 23.935 51.00 33.07 7.00 33.05 ATOM 2500 C GU THR 328 28.285 7.00 33.00 30.60 37.70 33.00 30.60 37.70 30.00 30.60 37.70 30.00 30.6									
ATOM 2478 CE2 PHE 324 20.146 58.105 28.542 1.00 37.79 ATOM 2490 C PHE 324 24.721 59.033 27.525 1.00 40.11 ATOM 2481 C PHE 324 24.721 59.033 27.525 1.00 40.11 ATOM 2481 C PHE 324 24.785 58.937 26.289 1.00 40.76 ATOM 2482 N GUU 325 25.129 58.072 28.350 1.00 39.06 ATOM 2483 C G GUU 325 25.129 58.072 28.350 1.00 39.06 ATOM 2483 C G GUU 325 25.740 56.851 27.844 1.00 37.85 ATOM 2484 C G GUU 325 26.846 56.418 28.781 1.00 38.17 ATOM 2487 C G GUU 325 27.790 57.528 29.085 1.00 40.68 ATOM 2487 C G GUU 325 28.922 57.705 29.951 1.00 40.68 ATOM 2489 C G GUU 325 28.653 56.608 31.086 1.00 44.06 ATOM 2489 C G GUU 325 28.653 56.608 31.086 1.00 44.06 ATOM 2489 C G GUU 325 28.653 56.608 31.086 1.00 44.06 ATOM 2489 C G GUU 325 28.922 57.705 29.951 1.00 40.68 ATOM 2489 C G GUU 325 28.925 57.705 29.840 1.00 36.60 ATOM 2489 C G GUU 325 29.903 55.445 28.447 1.00 37.31 ATOM 2491 N THR 326 25.019 54.958 26.554 1.00 35.30 ATOM 2492 CA THR 326 25.019 54.958 26.554 1.00 35.30 ATOM 2493 C G THR 326 24.935 33.816 26.255 1.00 31.58 ATOM 2493 C G THR 326 24.935 53.617 29.556 1.00 31.58 ATOM 2493 C G THR 326 24.935 53.617 29.556 1.00 31.58 ATOM 2493 C G THR 326 24.935 53.016 27.515 1.00 33.05 ATOM 2499 C G THR 326 24.935 53.016 27.515 1.00 33.05 ATOM 2499 C G THR 326 24.935 53.016 27.515 1.00 33.05 ATOM 2499 C G ARG 327 24.859 52.921 25.507 1.00 31.58 ATOM 2499 C G ARG 327 24.859 52.182 29.858 1.00 32.29 ATOM 2499 C G ARG 327 24.859 52.182 29.858 1.00 32.29 ATOM 2499 C G ARG 327 24.859 52.182 29.858 1.00 33.05 ATOM 2500 C ARG 327 27.596 51.043 32.177 1.00 38.88 ATOM 2501 C G ARG 327 26.146 52.245 30.417 1.00 33.30 ATOM 2501 C G ARG 327 27.596 51.043 32.177 1.00 38.88 ATOM 2501 C G ARG 327 27.596 51.043 32.177 1.00 38.88 ATOM 2501 C G ARG 327 27.596 51.043 32.177 1.00 38.88 ATOM 2501 C G ARG 327 27.596 51.043 32.277 1.00 38.88 ATOM 2501 C G ARG 327 27.596 51.043 32.277 1.00 38.88 ATOM 2501 C G ARG 327 27.596 51.043 32.277 1.00 38.88 ATOM 2501 C G ARG 327 28.865 51.663 31.669 1.00 27.73 ATOM 2501 C G ARG 327 28.865 51.663 31.669 1.00 27.73 ATOM 25									
ATOM 2499 C DHE 324 19.555 58.739 29.643 1.00 37.73 ATOM 2491 N PART 240 24.721 59.633 27.55 1.00 40.71 ATOM 2491 N GLU 325 25.129 58.072 28.350 1.00 39.66 ATOM 2498 C DHE 324 24.725 57.740 56.851 27.844 1.00 37.85 ATOM 2498 C DG DH 325 25.740 56.851 27.844 1.00 37.85 ATOM 2498 C DG DH 325 28.922 57.075 29.955 1.00 40.68 ATOM 2498 C DG DH 325 28.922 57.075 29.955 1.00 40.68 ATOM 2498 C DG DH 325 28.922 57.075 29.955 1.00 44.06 ATOM 2498 C DG DH 325 28.922 57.075 29.955 1.00 44.06 ATOM 2498 C DG DH 325 28.922 57.075 29.955 1.00 44.06 ATOM 2498 C DG DH 325 28.922 57.075 29.955 1.00 44.06 ATOM 2499 C DG DH 325 28.922 57.075 29.955 1.00 44.06 ATOM 2499 C DG DH 325 24.799 55.693 27.641 1.00 37.31 ATOM 2499 C DG DH 325 24.799 55.693 27.641 1.00 37.31 ATOM 2499 C DG DH 325 24.799 55.693 27.641 1.00 37.31 ATOM 2499 C DG DH 325 24.799 55.693 27.655 41.00 33.37 ATOM 2499 C DG DH 325 24.999 53.816 26.245 1.00 33.37 ATOM 2499 C DG DH 325 24.979 55.693 27.601 1.00 24.90 ATOM 2499 C DG DH 325 24.979 55.693 27.601 1.00 24.90 ATOM 2499 C DG DH 325 24.979 55.693 27.601 1.00 29.92 ATOM 2499 C DG DH 325 24.995 53.816 26.245 1.00 33.37 ATOM 2499 C DG THR 326 24.975 55.693 27.601 1.00 29.82 ATOM 2499 C DG THR 326 24.975 55.693 27.601 1.00 29.82 ATOM 2499 C DG THR 326 24.975 55.001 30.805 57.181 29.901 30.805 57.495 50.001 30.305 50.001 30.901 30									
ATOM 2480 C PHE 324									
ATOM 2481 Q									
ATOM 2482 N GLU 325									
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ATOM 2491 N THR 326			С			24.799	55.693	27.641	1.00 36.60
ATOM 2492 CA THR 326	MOTA	2490	0	GLU	325	23.903	55.445	28.447	1.00 37.31
ATOM 2499 CB THR 326						25.019	54.968	26.554	1.00 35.30
ATOM 2494 OCI THR 326 24.934 53.617 23.956 1.00 29.94 ATOM 2495 CC THR 326 22.915 53.016 27.515 1.00 33.05 ATOM 2497 O THR 326 22.946 52.528 27.742 1.00 33.05 ATOM 2497 O THR 326 22.946 52.528 27.742 1.00 33.05 ATOM 2498 N ARG 327 24.859 52.148 29.588 1.00 31.76 ATOM 2499 CA ARG 327 24.859 52.148 29.588 1.00 31.76 ATOM 2499 CA ARG 327 24.859 52.148 29.588 1.00 31.76 ATOM 2500 CB ARG 327 24.859 52.148 29.588 1.00 31.76 ATOM 2500 CB ARG 327 24.859 52.148 29.588 1.00 31.76 ATOM 2501 CA ARG 327 24.859 52.148 29.588 1.00 31.76 ATOM 2501 CA ARG 327 27.596 51.162 31.465 1.00 36.71 ATOM 2502 CD ARG 327 27.596 51.162 31.465 1.00 36.71 ATOM 2503 NB ARG 327 27.596 51.043 32.177 1.00 38.88 ATOM 2504 CZ ARG 327 28.5146 52.5245 30.147 1.00 30.621 ATOM 2505 NB ARG 327 27.595 52.024 33.249 1.00 40.62 ATOM 2505 NB ARG 327 28.515 33.059 1.00 41.13 ATOM 2505 NB ARG 327 28.615 53.670 31.846 1.00 40.49 ATOM 2505 NB ARG 327 28.615 53.670 31.846 1.00 40.49 ATOM 2505 NB ARG 327 23.681 52.691 30.387 1.00 30.52 ATOM 2507 N PHB 328 22.535 30.4078 34.113 1.00 40.82 ATOM 2507 N PHB 328 22.535 954.014 30.425 1.00 29.96 ATOM 2507 CA ARG 327 23.681 52.691 30.387 1.00 30.52 ATOM 2507 CA ARG 327 23.681 52.691 30.387 1.00 30.52 ATOM 2507 CA ARG 327 23.681 52.691 30.387 1.00 30.52 ATOM 2507 CA PHB 328 22.479 54.663 31.154 1.00 28.70 ATOM 2510 CA PHB 328 22.479 54.663 31.154 1.00 28.70 ATOM 2510 CA PHB 328 22.479 54.663 31.454 1.00 28.70 ATOM 2510 CA PHB 328 22.479 54.663 31.491 1.00 27.73 ATOM 2512 CG PHB 328 22.479 54.663 31.591 1.00 28.70 ATOM 2515 CE PHB 328 24.678 55.857 32.555 1.00 29.95 ATOM 2510 CA PHB 328 25.526 58.437 31.992 1.00 28.74 ATOM 2510 CA PHB 328 25.526 58.437 31.992 1.00 28.74 ATOM 2510 CA PHB 328 25.526 58.437 31.992 1.00 28.75 ATOM 2510 CA PHB 328 25.526 58.437 31.992 1.00 28.75 ATOM 2510 CA PHB 328 25.526 58.437 31.592 1.00 28.75 ATOM 2510 CA PHB 328 25.526 58.437 31.992 1.00 28.75 ATOM 2510 CA PHB 328 25.526 58.437 31.992 1.00 28.75 ATOM 2510 CA PHB 328 25.526 58.437 31.992 1.00 28.75 ATOM 2510 CA PHB 328 25.526 58.437 31.			CA	THR	326	24.193	53.816	26.245	1.00 33.37
ATOM 2495 CG2 THR 326 24,113 51,619 25,041 1.00 29,94 ATOM 2496 C THR 326 23,951 53,016 27,755 1.00 33,05 ATOM 2497 O THR 326 22,946 52,282 27,742 1.00 33,05 ATOM 2499 N ARG 327 24,881 52,292 28,349 1.00 32,29 ATOM 2501 CG ARG 327 26,146 52,245 30,417 1.00 33,30 ATOM 2501 CG ARG 327 26,146 52,245 30,417 1.00 33,30 ATOM 2503 NE ARG 327 27,596 51,043 32,177 1.00 38,98 ATOM 2504 CZ ARG 327 28,274 53,255 33,069 1.00 41,13 ATOM 2505 NPI JARG 327 <t< td=""><td>MOTA</td><td>2493</td><td>CB</td><td>THR</td><td>326</td><td>24.875</td><td>52.921</td><td>25.207</td><td>1.00 31.58</td></t<>	MOTA	2493	CB	THR	326	24.875	52.921	25.207	1.00 31.58
ATOM 2495 CG THR 326 24.113 51.619 25.041 1.00 29.94 ATOM 2497 C THR 326 23.951 53.016 27.515 1.00 33.05 ATOM 2497 C THR 326 22.846 52.528 27.762 1.00 33.05 ATOM 2499 N ARG 327 24.859 52.128 29.762 1.00 33.95 ATOM 2499 N ARG 327 24.859 52.128 29.92 28.349 1.00 31.76 ATOM 2500 CB ARG 327 26.126 52.252 30.417 1.00 33.30 ATOM 2501 CG ARG 327 26.126 52.253 30.417 1.00 33.30 ATOM 2501 CG ARG 327 26.126 52.253 30.417 1.00 33.30 ATOM 2503 NE ARG 327 27.956 51.023 32.177 1.00 38.88 ATOM 2505 NR1 ARG 327 27.956 52.024 33.249 1.00 40.62 ATOM 2505 NR1 ARG 327 28.615 53.650 31.49 1.00 40.62 ATOM 2505 NR1 ARG 327 28.615 53.600 31.76 ATOM 2507 C ARG 327 28.615 53.600 31.866 1.00 40.49 ATOM 2508 O ARG 327 22.888 51.930 30.940 1.00 29.95 ATOM 2509 N PHE 328 22.559 54.014 30.255 1.00 28.70 ATOM 2510 CA PHE 328 22.559 54.014 30.255 1.00 28.70 ATOM 2511 CB PHE 328 22.632 56.176 31.069 1.00 28.70 ATOM 2512 CG PHE 328 22.632 56.176 31.069 1.00 28.03 ATOM 2513 CD PHE 328 24.678 55.887 32.555 1.00 28.92 ATOM 2516 CE PHE 328 22.632 56.176 31.069 1.00 28.03 ATOM 2516 CE PHE 328 22.632 56.176 31.069 1.00 28.03 ATOM 2516 CE PHE 328 22.632 56.176 31.069 1.00 28.03 ATOM 2516 CE PHE 328 22.632 56.176 31.069 1.00 28.03 ATOM 2516 CE PHE 328 22.632 56.176 31.069 1.00 28.03 ATOM 2517 CZ PHE 328 25.526 58.437 31.992 1.00 28.73 ATOM 2518 C PHE 328 25.871 56.305 33.069 1.00 28.74 ATOM 2519 O PHE 328 25.871 56.305 33.069 1.00 28.74 ATOM 2510 CE PHE 328 26.298 57.599 32.812 1.00 28.68 ATOM 2520 C VAL 329 19.830 53.755 28.587 1.00 26.44 ATOM 2521 CA VAL 329 19.830 53.755 28.587 1.00 26.44 ATOM 2522 CB VAL 329 19.830 53.755 29.576 1.00 27.98 ATOM 2522 CB VAL 329 19.830 53.755 29.576 1.00 27.98 ATOM 2525 C VAL 329 19.800 53.755 29.579 1.00 28.76 ATOM 2525 C VAL 329 19.800 53.755 29.579 1.00 28.76 ATOM 2525 C VAL 329 19.800 53.755 29.579 1.00 28.76 ATOM 2525 C VAL 329 19.800 53.755 29.579 1.00 28.76 ATOM 2525 C VAL 329 19.800 53.755 29.579 1.00 28.76 ATOM 2525 C VAL 329 19.800 53.755 29.591 1.00 28.76 ATOM 2525 C VAL 329 19.800 53.755 29.591 1.00 28.76	ATOM	2494	OG1	THR	326	24.934	53.617	23.956	1.00 29.82
ATOM 2496 C THR 326 23,951 53,016 27,515 1.00 33.05 ATOM 2497 O THR 326 22,846 52,528 27,772 1.00 33.09 ATOM 2498 N ARG 327 24,981 52,902 28,349 1.00 32.29 ATOM 2501 CG ARG 327 24,859 52,148 29,588 1.00 31.76 ATOM 2501 CG ARG 327 25,146 52,248 30,417 1.00 33.30 ATOM 2501 CC ARG 327 27,795 52,044 33,249 1.00 40.62 ATOM 2504 CZ ARG 327 28,615 53,670 31,846 1.00 40.49 ATOM 2506 NE2 ARG 327 28,615 53,670 31,846 1.00 40.49 ATOM 2508 N RRG 327 </td <td>MOTA</td> <td>2495</td> <td>CG2</td> <td>THR</td> <td>326</td> <td>24.113</td> <td></td> <td>25.041</td> <td>1.00 29.94</td>	MOTA	2495	CG2	THR	326	24.113		25.041	1.00 29.94
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ATOM 2531 C SER 330 19.534 50.107 31.172 1.00 31.40									
ATOM 2532 O SER 330 18.690 49.298 31.577 1.00 31.74									
	ATOM	2532	0	SER	330	18.690	49.298	31.577	1.00 31.74

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ATOM	2533	N	GLN	331	20 110	50.000	24 000	15
ATOM	2534	CA	GLN	331	20.118	50.993	31.972	1.00 32.45
ATOM	2535	CB	GLN	331	19.745 20.668	51.061	33.381	1.00 33.16
MOTA	2536	CG	GLN	331	22.093	51.992	34.151	1.00 33.58
ATOM	2537	CD	GLN	331		51.540	34.194	1.00 35.83
ATOM	2538		GLN		22.947	52.534	34.919	1.00 37.72
				331	22.626	52.927	36.043	1.00 39.62
ATOM	2539		GLN	331	24.042	52.958	34.291	1.00 38.98
MOTA	2540	С	GLN	331	18.327	51.591	33.482	1.00 33.78
MOTA	2541	0	GLN	331	17.428	50.881	33.938	1.00 34.06
MOTA	2542	N	VAL	332	18.129	52.835	33.038	1.00 33.77
MOTA	2543	CA	VAL	332	16.808	53.457	33.097	1.00 33.65
MOTA	2544	CB	VAL	332	16.760	54.791	32.282	1.00 32.19
MOTA	2545	CG1	VAL	332	17.279	54.584	30.905	1.00 33.04
MOTA	2546	CG2	VAL	332	15.340	55.312	32.215	1.00 31.67
MOTA	2547	C	VAL	332	15.695	52.505	32.638	1.00 34.20
MOTA	2548	0	VAL	332	14.571	52.566	33.139	1.00 34.51
MOTA	2549	N	GLU	333	16.001	51.607	31.711	1.00 34.30
MOTA	2550	CA	GLU	333	14.981	50.676	31.258	1.00 34.92
MOTA	2551	CB	GLU	333	15.210	50.289	29.795	1.00 34.40
MOTA	2552	CG	GLU	333	14.893	51.413	28.837	1.00 33.07
MOTA	2553	CD	GLU	333	14.806	50.956	27.409	1.00 31.80
MOTA	2554		GLU	333	13.983	50.060	27.114	1.00 31.65
MOTA	2555		GLU	333	15.561	51.504	26.581	1.00 31.72
MOTA	2556	С	GLU	333	14.949	49.438	32.135	1.00 35.76
MOTA	2557	0	GLU	333	14.163	48.520	31.911	1.00 35.73
MOTA	2558	N	SER	334	15.814	49.419	33.138	1.00 36.91
MOTA	2559	CA	SER	334	15.876	48.307	34.071	1.00 38.13
MOTA	2560	CB	SER	334	17.328	47.934	34.346	1.00 39.38
MOTA	2561	OG	SER	334	17.460	46.524	34.468	1.00 41.52
MOTA	2562	С	SER	334	15.201	48.747	35.362	1.00 37.93
ATOM	2563	0	SER	334	15.053	47.973	36.306	1.00 38.63
MOTA	2564	N	ASP	335	14.807	50.014	35.385	1.00 38.51
ATOM	2565	CA	ASP	335	14.133	50.619	36.521	1.00 38.59
ATOM	2566	CB	ASP	335	13.776	52.061	36.173	1.00 39.10
ATOM	2567	CG	ASP	335	13.346	52.864	37.373	1.00 39.89
MOTA	2568		ASP	335	12.278	52.547	37.950	1.00 40.30
MOTA	2569		ASP	335	14.079	53.816	37.737	1.00 39.90
MOTA	2570	С	ASP	335	12.876	49.809	36.840	1.00 39.11
MOTA	2571	0	ASP	335	12.241	49.249	35.945	1.00 39.03
MOTA	2572	N	THR	336	12.517	49.768	38.119	1.00 39.68
MOTA	2573	CA	THR	336	11.372	48.999	38.605	1.00 39.94
MOTA	2574	CB	THR	336	11.773	48.297	39.896	1.00 39.68
MOTA	2575	0G1	THR	336	12.901	47.464	39.630	1.00 40.95
MOTA	2576	CG2	THR	336	10.650	47.452	40.425	1.00 39.84
MOTA	2577	С	THR	336	10.043	49.735	38.853	1.00 40.52
MOTA	2578	0	THR	336	8.984	49108	38.931	1.00 40.91
MOTA	2579	N	GLY	337	10.085	51.054	38.970	1.00 40.80
MOTA	2580	CA	GLY	337	8.870	51.804	39.234	1.00 41.83
ATOM	2581	С	GLY	337	9.307	52.948	40.112	1.00 42.60
ATOM	2582	0	GLY	337	8.990	54.105	39.865	1.00 43.33
ATOM	2583	N	ASP	338	10.043	52.604	41.156	1.00 43.47
ATOM	2584	CA	ASP	338	10.606	53.589	42.059	1.00 44.40
ATOM	2585	CB	ASP	338	11.354	52.868	43.175	1.00 44.83
ATOM	2586	CG	ASP	338	12.303	51.808	42.637	1.00 45.34
ATOM	2587		ASP	338	11.879	51.032	41.751	1.00 46.12
MOTA	2588	OD2	ASP	338	13.465	51.742	43.087	1.00 45.59
MOTA	2589	С	ASP	338	11.597	54.296	41.142	1.00 44.84
MOTA	2590	0	ASP	338	12.605	53.709	40.756	1.00 45.53
MOTA	2591	N	ARG	339	11.310	55.533	40.763	1.00 44.81

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MOTA	2592	CA	ARG	339	10.000			
ATOM	2593				12.208	56.256	39.874	1.00 45.11
		CB	ARG	339	11.702	57.687	39.654	1.00 45.72
ATOM	2594	CG	ARG	339	10.466	57.799	38.783	1.00 46.11
ATOM	2595	CD	ARG	339	9.201	57.413	39.521	1.00 46.99
MOTA	2596	NΞ	ARG	339	8.041	57.492	38.633	1.00 47.58
ATOM	2597	CZ	ARG	339	6.780	57.326	39.017	1.00 47.30
ATOM	2598	NH1	ARG	339	6.492	57.068	40.287	1.00 47.38
MOTA	2599	NH2	ARG	339	5.806	57.413	38.123	1.00 47.44
MOTA	2600	С	ARG	339	13.637	56.295	40.419	1.00 44.98
MOTA	2601	0	ARG	339	14.466	57.084	39.960	1.00 44.83
MOTA	2602	N	LYS	340	13.922	55.441	41.394	1.00 44.75
MOTA	2603	CA	LYS	340	15.238	55.394	42.001	1.00 45.05
MOTA	2604	CB	LYS	340	15.341	54.179	42.917	1.00 46.19
MOTA	2605	CG	LYS	340	14.358	54.250	44.081	1.00 47.87
ATOM	2606	CD	LYS	340	14.598	53.154	45.094	1.00 49.25
MOTA	2607	CE	LYS	340	13.365	52.949	45.957	1.00 50.44
ATOM	2608	NZ	LYS	340	13.353	51.589	46.598	1.00 51.78
ATOM	2609	C	LYS	340	16.398	55.422	41.014	1.00 44.66
ATOM	2610	0	LYS	340	17.186	56.372	41.026	1.00 44.90
ATOM	2611	N	GLN	341	16.509	54.408	40.155	1.00 43.94
ATOM	2612	CA	GLN	341	17.603	54.362	39.174	1.00 42.93
MOTA	2613	CB	GLN	341	17.598	53.028	38.435	1.00 45.04
ATOM	2614	CG	GLN	341	18.035	51.860	39.289	1.00 48.03
ATOM	2615	CD	GLN	341	18.758	50.801	38.482	1.00 49.69
ATOM	2616	0E1	GLN	341	19.731	51.101	37.779	1.00 50.67
ATOM	2617	NE2	GLN	341	18.297	49.556	38.581	1.00 50.67
ATOM	2618	C	GLN	341	17.616	55.497		
ATOM	2619	ō	GLN	341	18.672	56.057	38.146	1.00 40.93
ATOM	2620	N	ILE	342	16.449	55.824	37.839	1.00 38.85
ATOM	2621	CA	ILE	342	16.364		37.600	1.00 39.61
ATOM	2622	CB	ILE	342	14.920	56.905	36.624	1.00 39.07
ATOM	2623	CG2	ILE	342		57.110	36.130	1.00 39.24
ATOM	2624	CG1	ILE	342	14.880	58.226	35.107	1.00 39.19
MOTA	2625	CD1	ILE	342	14.392	55.817	35.501	1.00 39.87
ATOM	2626	C	ILE	342	12.945	55.902	35.070	1.00 40.76
ATOM	2627	ō	ILE	342	16.832	58.185	37.301	1.00 38.43
ATOM	2628	N	TYR	343	17.704	58.892	36.795	1.00 37.48
ATOM	2629	CA	TYR	343	16.240	58.466	38.456	1.00 38.93
ATOM	2630	CB	TYR	343	16.580	59.647	39.236	1.00 39.71
ATOM	2631	CG	TYR	343	15.813	59.656	40.567	1.00 40.97
ATOM	2632	CD1	TYR	343	16.173	60.835	41.448	1.00 42.53
ATOM	2633	CE1	TYR	343	15.344	61.954	41.521	1.00 43.30
ATOM	2634	CD2	TYR	343	15.730	63.092	42.228	1.00 44.58
ATOM	2635	CE2	TYR	343	17.397	60.880	42.119	1.00 43.04
ATOM	2636	CZ	TYR		17.791	62.014	42,.826	1.00 43.55
ATOM	2637	OH		343	16.958	63.117	42.872	1.00 44.31
ATOM	2638		TYR	343	17.369	64.260	43.523	1.00 45.74
ATOM	2639	C	TYR	343	18.070	59.635	39.532	1.00 39.93
ATOM	2640	N	TYR	343	18.789	60.598	39.262	1.00 40.28
				344	18.525	58.529	40.098	1.00 40.14
ATOM	2641	CA	ASN	344	19.924	58.371	40.460	1.00 40.97
ATOM	2642	CB	ASN	344	20.146	56.958	40.989	1.00 42.94
ATOM	2643	CG	ASN	344	21.287	56.880	41.977	1.00 44.68
ATOM	2644	OD1	ASN	344	22.448	57.137	41.628	1.00 46.05
ATOM	2645		ASN	344	20.965	56.531	43.225	1.00 44.93
MOTA	2646	C	ASN	344	20.869	58.649	39.292	1.00 40.46
ATOM	2647	0	ASN	344	21.946	59.208	39.483	1.00 40.33
MOTA	2648	N	ILE	345	20.460	58.262	38.085	1.00 40.50
MOTA	2649	CA	ILE	345	21.280	58.467	36.890	1.00 39.89
ATCM	2650	CB	ILE	345	20.803	57.555	35.720	1.00 39.76

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ATOM	2651	CC2	ILE	345	21.597	57.849	24 440	1.00 38.62
MOTA	2652	CG1	ILE	345	20.966		34.448	
MOTA		CD1		345		56.090	36.114	1.00 38.74
	2653		ILE		20.201	55.151	35.242	1.00 38.61
ATOM	2654	C	ILE	345	21.247	59.924	36.434	1.00 39.80
MOTA	2655	0	ILE	345	22.281	60.490	36.074	1.00 39.67
MOTA	2656	N	LEU	346	20.062	60.529	36.449	1.00 39.59
MOTA	2657	CA	LEU	346	19.912	61.923	36.029	1.00 39.58
MOTA	2658	CB	LEU	346	18.434	62.255	35.818	1.00 37.79
MOTA	2659	CG	LEU	346	17.809	61.528	34.625	1.00 36.58
MOTA	2660		LEU	346	16.277	61.599	34.684	1.00 35.18
ATOM	2661		LEU	346	18.363	62.145	33.337	1.00 35.05
MOTA	2662	С	LEU	346	20.519	62.892	37.034	1.00 40.82
ATOM	2663	0	LEU	346	21.177	63.857	36.654	1.00 41.02
ATOM	2664	N	SER	347	20.298	62.646	38.322	1.00 42.34
MOTA	2665	CA	SER	347	20.859	63.530	39.339	1.00 43.44
MOTA	2666	CB	SER	347	20.491	63.042	40.745	1.00 43.90
ATOM	2667	OG	SER	347	20.665	61.639	40.868	1.00 45.32
ATOM	2668	С	SER	347	22.368	63.556	39.156	1.00 43.44
ATOM	2669	0	SER	347	22.974	64.624	39.051	1.00 44.11
ATOM	2670	N	THR	348	22.969	62.374	39.096	1.00 43.10
ATOM	2671	CA	THR	348	24,407	62.285	38.909	1.00 42.97
ATOM	2672	CB	THR	348	24.853	60.830	38.700	1.00 42.31
ATOM	2673	OG1		348	24.666	60.096	39.918	1.00 42.08
ATOM	2674	CG2	THR	348	26.322	60.780	38.282	1.00 40.85
MOTA	2675	C	THR	348	24.798	63.093	37.683	1.00 43.25
ATOM	2676	Ö	THR	348	25.796			
ATOM	2677	N	LEU	349		63.813	37.680	1.00 43.52
MOTA	2678	CA	LEU	349	23.990 24.271	62.982	36.640	1.00 43.57
ATOM	2679	CB	LEU	349		63.697	35.412	1.00 44.17
MOTA	2680	CG	LEU	349	23.343	63.180	34.311	1.00 44.43
ATOM					23.787	63.204	32.847	1.00 44.86
	2681		LEU	349	25.198	62.658	32.688	1.00 44.59
MOTA	2682		LEU	349	22.790	62.375	32.046	1.00 44.64
ATOM	2683	C	LEU	349	24.102	65.201	35.638	1.00 44.32
MOTA	2684	0	LEU	349	24.317	66.003	34.726	1.00 45.33
ATOM	2685	N	GLY	350	23.722	65.574	36.862	1.00 43.94
ATOM	2686	CA	GLY	350	23.559	66.981	37.210	1.00 43.15
ATOM	2687	C	GLY	350	22.167	67.570	37.038	1.00 42.49
ATOM	2688	0	GLY	350	22.024	68.752	36.703	1.00 41.70
ATOM	2639	N	LEU	351	21.143	66.758	37.288	1.00 41.97
ATOM	2690	CA	LEU	351	19.758	67.197	37.132	1.00 41.45
ATOM	2691	СB	LEU	351	19.194	66.676	35.812	1.00 40.99
ATCM	2692	CG	LEU	351	19.875	67.115	34.522	1.00 40.66
ATOM	2693	CD1	LEU	351	19.516	66.144	33.416	1.00 41.63
ATOM	2694	CD2	LEU	351	19.453	68.533	34.172	1.00 40.77
ATOM	2695	С	LEU	351	18.858	66.718	38.262	1.00 41.15
ATOM	2696	0	LEU	351	19.170	65760	38.973	1.00 40.88
ATOM	2697	N	ARG	352	17.720	67.379	38.410	1.00 41.10
ATOM	2698	CA	ARG	352	16.782	67.007	39.457	1.00 41.25
ATOM	2699	CB	ARG	352	16.614	68.173	40.431	1.00 42.65
ATOM	2700	CG	ARG	352	17.929	68.581	41.070	1.00 43.68
ATOM	2701	CD	ARG	352	18.504	67.421	41.851	1.00 45.59
ATOM	2702	NE	ARG	352	19.960	67.478	41.917	1.00 47.73
ATOM	2703	CZ	ARG	352	20.715	66.567	42.521	1.00 48.77
MOTA	2704	NH1	ARG	352	20.143	65.524	43.119	1.00 49.05
ATOM	2705	NH2	ARG	352	22.038	66.700	42.519	1.00 49.14
ATOM	2706	C	ARG	352	15.458	66.621	38.827	1.00 39.59
ATOM	2707	0	ARG	352	14.512	67.399	38.793	1.00 40.34
MOTA	2708	N	PRO	353	15.378	65.388	38.324	1.00 38.06
ATOM	2709	CD	PRO	353	16.325	64.285	38.555	1.00 37.28
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MOTA	2710	CA	PRO	353	14.159	64.901	37.683	1.00 37.45
ATOM	2711	CB	PRO	353	14.139	63.552	37.134	1.00 37.43
MOTA	2712	CG	PRO	353				1.00 36.92
ATOM			PRO	353	15.491	63.064	38.232	
	2713	C			12.998	64.763	38.650	1.00 36.35
MOTA	2714	0	PRO	353	13.180	64.360	39.791	1.00 36.28
ATOM	2715	N	SER	354	11.805	65.110	38.194	1.00 35.82
MOTA	2716	CA	SER	354	10.625	64.951	39.028	1.00 36.40
ATOM	2717	CB	SER	354	9.570	66.010	38.698	1.00 35.94
MOTA	2718	OG	SER	354	8.944	65.725	37.459	1.00 35.63
MOTA	2719	С	SER	354	10.091	63.570	38.653	1.00 36.41
MOTA	2720	0	SER	354	10.592	62.948	37.716	1.00 37.42
MOTA	2721	N	THR	355	9.087	63.091	39.375	1.00 36.02
MOTA	2722	CA	THR	355	8.493	61.790	39.099	1.00 35.68
MOTA	2723	CB	THR	355	7.200	61.615	39.923	1.00 36.38
ATOM	2724	OG1	THR	355	7.525	61.645	41.316	1.00 37.75
ATOM	2725	CG2	THR	355	6.510	60.293	39.598	1.00 36.44
MOTA	2726	C	THR	355	8.161	61.633	37.609	1.00 35.80
ATOM	2727	0	THR	355	8.319	60.548	37.029	1.00 34.73
MOTA	2728	N	THR	356	7.698	62.720	36.994	1.00 35.28
ATOM	2729	CA	THR	356	7.336	62.690	35.586	1.00 35.39
ATOM	2730	CB	THR	356	6.287	63.774	35.263	1.00 35.59
ATOM	2731	OG1	THR	356	6.651	64.990	35.925	1.00 35.39
ATOM	2732	CG2	THR	356	4.892	63.331	35.719	1.00 34.33
ATOM	2733	C	THR	356	8.542	62.848	34.662	1.00 35.30
ATOM	2734	ō	THR	356	8.560	62.285	33.559	1.00 34.91
MOTA	2735	N	ASP	357	9.537	63.624	35.089	1.00 35.07
ATOM	2736	CA	ASP	357	10.740	63.782	34.277	1.00 35.80
ATOM	2737	CB	ASP	357	11.804	64.598	35.012	1.00 36.76
ATOM	2738	CG	ASP	357	11.451	66.077	35.116	1.00 38.19
ATOM	2739	OD1	ASP	357	11.475	66.778	34.071	1.00 37.60
ATOM	2740	OD2	ASP	357	11.475	66.538	36.249	1.00 37.00
MOTA	2741	C	ASP	357	11.138	62.373	34.039	1.00 35.70
MOTA	2742	o	ASP	357	11.460	61.942	32.901	1.00 36.94
ATOM	2742	N	CYS	358	11.498			1.00 35.67
ATOM	2744	CA	CYS	358	12.013	61.649	35.131	1.00 35.44
ATOM	2745	CB	CYS	358	12.013	60.293	35.057	1.00 35.44
ATOM	2745	SG	CYS	358		59.658	36.447	
ATOM	2747	C	CYS	358	13.247 11.177	60.410	37.575	1.00 35.81
ATOM	2748	o	CYS	358	11.711	59.433	34.138	1.00 34.88
ATOM	2749	N	ASP	359		58.698	33.308	1.00 35.87
ATOM	2750	CA	ASP	359	9.863	59.517	34.290	
MOTA	2751	CB	ASP	359	8.960	58.729	33.464	1.00 33.10
ATOM	2752	CG			7.519	58.964	33.910	1.00 35.03
ATOM	2753		ASP	359 359	7.118	58.058	35.062	1.00 36.65
		OD2			7.950	57.850	35.975	1.00 38.15
ATOM	2754	C C		359	5.969	57.561	35.055	1.00 37.12
MOTA MOTA	2755		ASP	359	9.130	59 -058	31.985	1.00 31.16
	2756	0	ASP	359	9.090	58.170	31.133	1.00 30.01
ATOM	2757	N	ILE	360	9325	60.334	31.682	1.00 29.54
ATOM	2758	CA	ILE	360	9.524	60.741	30.300	1.00 28.61
ATOM	2759	CB	ILE	360	9.546	62.273	30.162	1.00 27.75
ATOM	2760	CG2		360	10.255	62.668	28.874	1.00 27.01
ATOM	2761	CG1		360	8.112	62.818	30.235	1.00 26.18
ATOM	2762		ILE	360	8.024	64.322	30.190	1.00 23.23
ATOM	2763	C	ILE	360	10.857	60.176	29.825	1.00 29.21
MOTA	2764	0	ILE	360	10.919	59.480	28.805	1.00 29.88
ATOM	2765	N	VAL	361	11.923	60.466	30.569	1.00 28.39
MOTA	2766	CA	VAL	361	13.248	59.971	30.219	1.00 28.01
ATOM	2767	CB	VAL	361	14.258	60.256	31.342	1.00 27.73
ATOM	2768	CG1	VAL	361	15.575	59.551	31.055	1.00 27.43

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ATOM	2769	000	VAL	361	1.4.400			
MOTA	2770	C	VAL	361	14.492 13.245	61.759	31.453	1.00 27.76
MOTA	2771	ō	VAL	361	14.055	58.464 57.982	29.919 29.107	1.00 27.74
MOTA	2772	N	ARG	362	12.341	57.719	30.556	1.00 27.40
ATOM	2773	CA	ARG	362	12.277	56.275	30.325	1.00 27.72
ATOM	2774	CB	ARG	362	11.523	55.571	31.455	1.00 27.93
ATOM	2775	CG	ARG	362	11.137	54.147	31.101	1.00 31.97
MOTA	2776	CD	ARG	362	10.900	53.266	32.308	1.00 33.93
MOTA	2777	NE	ARG	362	10.930	51.859	31.893	1.00 37.37
MOTA	2778	CZ	ARG	362	10.938	50.817	32.725	1.00 37.52
MOTA	2779	NH1	ARG	362	10.920	51.010	34.043	1.00 38.72
MOTA	2780	NH2	ARG	362	10.960	49.582	32.230	1.00 36.06
MOTA	2781	С	ARG	362	11.614	55.959	28.994	1.00 27.88
MOTA	2782	0	ARG	362	12.016	55.032	28.289	1.00 29.02
ATOM	2783	N	ARG	363	10.586	56.728	28.660	1.00 27.31
ATOM	2784	CA	ARG	363	9.866	56.564	27.400	1.00 25.77
MOTA	2785	CB	ARG	363	8.641	57.486	27.374	1.00 26.51
MOTA	2786	CG	ARG	363	7.530	57.084	28.318	1.00 26.30
ATOM	2787	CD	ARG	363	6.730	55.929	27.739	1.00 28.36
MOTA	2788	NE	ARG	363	6.259	56.216	26.380	1.00 30.91
ATOM	2789 2790	CZ	ARG	363 363	6.872	55.826	25.260	1.00 31.55
MOTA	2791		ARG	363	7.992 6.370	55.112	25.315	1.00 33.18
ATOM	2792	C	ARG	363	10.817	56.158 56.949	24.077	1.00 32.30
ATOM	2793	Ö	ARG	363	10.748	56.392	25.175	1.00 24.71
MOTA	2794	N	ALA	364	11.706	57.905	26.540	1.00 23.90
MOTA	2795	CA	ALA	364	12.653	58.339	25.507	1.00 24.48
MOTA	2796	CB	ALA	364	13.463	59.545	25.969	1.00 23.15
MOTA	2797	C	ALA	364	13.571	57.176	25.226	1.00 25.01
ATOM	2798	0	ALA	364	13.854	56.872	24.069	1.00 26.22
ATOM	2799	N	CYS	365	14.023	56.518	26.290	1.00 25.03
MOTA	2800	CA	CYS	365	14.902	55.370	26.157	1.00 24.77
MOTA	2801	СВ	CYS	365	15.450	54.970	27.528	1.00 23.03
ATOM	2802	SG	CYS	365	16.728	56.114	28.173	1.00 21.60
MOTA	2803	C	CYS	365	14.140	54.206	25.514	1.00 25.44
MOTA	2804	0	CYS	365	14.661	53.535	24.617	1.00 27.49
ATOM	2805 2806	N CA	GLU	366 366	12.906	53.956	25.944	1.00 26.87
MOTA	2807	CB	GLU	366	12.145 10.757	52.859 52.743	25.342 25.988	1.00 27.98 1.00 28.74
MOTA	2808	CG	GLU	366	10.785	52.743	27.490	1.00 28.74
ATOM	2809	CD	GLU	366	9.427	51.981	28.041	1.00 30.75
ATOM	2810	0E1	GLU	366	8.444	52.757	27.970	1.00 32.39
ATOM	2811	OE2	GLU	366	9.342	50.841	28.547	1.00 33.30
ATOM	2812	C	GLU	366	12.005	53.056	23,815	1.00 28.15
MOTA	2813	0	GLU	366	12.117	52.104	23.029	1.00 27.63
MOTA	2814	N	SER	367	11.776	54.304	23.407	1.00 28.42
MOTA	2815	CA	SER	367	11.612	54.650	21.993	1.00 27.23
MOTA	2816	CB	SER	367	11.368	56.156	21.833	1.00 27.45
MOTA	2817	OG	SER	367	10.161	56.552	22.447	1.00 27.44
MOTA	2818	C	SER	367	12.824	54.276	21.165	1.00 26.52
MOTA	2819	0	SER	367	12.724	53.567	20.162	1.00 27.99
MOTA	2820 2821	N CA	VAL	368	13.977	54.773	21.581	1.00 24.30
ATOM	2821	CB	VAL	368 368	15.194 16.324	54.499	20.849	1.00 22.45
ATOM	2823	CG1	VAL	368	17.623	55.395	21.375	1.00 20.96
ATOM	2824	CG2	VAL	368	15.928	55.075 56.843	20.682	1.00 18.44
ATOM	2825	C	VAL	368	15.605	53.019	20.888	1.00 23.13
MOTA	2826	ō	VAL	368	15.850	52.420	19.832	1.00 23.13
ATOM	2827	N	SER	369	15.660	52.405	22.071	1.00 22.54
					_5.550	-2.403		2.00 22.32

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ATOM	2828	CA	SER	369	16.071	51.003	22.106	1.00 21.93
ATOM	2829	CB	SER	369	16.248	50.476	23.542	1.00 23.39
ATOM	2830	OG	SER	369	15.011	50.251	24.197	1.00 25.91
ATOM	2831	C	SER	369	15.109	50.112	21.348	1.00 20.54
ATOM	2832	0	SER	369	15.526	49.063	20.850	1.00 20.31
ATOM	2833	N	THR	370	13.832	50.499	21.259	1.00 18.40
ATOM	2834	CA	THR	370	12.878	49.682	20.496	1.00 17.32
ATOM	2835	CB	THR	370	11.400	49.976	20.859	1.00 16.46
ATOM	2836	OG1	THR	370	11.053	49.298	22.073	1.00 15.81
MOTA MOTA	2837 2838	CG2	THR	370	10.473	49.487	19.774	1.00 14.39
ATOM	2839	C O	THR	370 370	13.076	49.936	19.001	1.00 17.03
ATOM	2840	N	THR	370	12.977	49.008	18.186	1.00 17.38
ATOM	2841	CA	ARG	371	13.358 13.562	51.177	18.617	1.00 16.71
ATOM	2842	CB	ARG	371		51.423	17.201	1.00 16.54
ATOM	2843	CG	ARG	371	13.810 14.013	52.905	16.882	1.00 17.42
ATOM	2844	CD	ARG	371	14.013	53.123	15.374	1.00 17.76
ATOM	2845	NE	ARG	371	15.567	54.559 55.076	14.943	1.00 17.40
ATOM	2846	CZ	ARG	371	16.159		15.412	
ATOM	2847	NH1	ARG	371	15.583	56.154 56.810	14.896 13.892	1.00 18.99
ATOM	2848		ARG	371	17.303	56.605	15.406	1.00 17.43
ATOM	2849	С	ARG	371	14.763	50.607	16.759	1.00 15.15
ATOM	2850	ō	ARG	371	14.689	49.929	15.748	1.00 17.14
ATOM	2851	N	ALA	372	15.856	50.644	17.519	1.00 15.40
ATOM	2852	CA	ALA	372	17.061	49.883	17.148	1.00 16.23
ATOM	2853	CB	ALA	372	18.152	50.046	18.197	1.00 15.66
ATOM	2854	С	ALA	372	16.775	48.407	16.957	1.00 16.83
ATOM	2855	0	ALA	372	17.125	47.838	15.923	1.00 18.06
MOTA	2856	N	ALA	373	16.149	47.790	17.955	1.00 16.86
ATOM	2857	CA	ALA	373	15.817	46.367	17.912	1.00 17.10
ATOM	2858	CB	ALA	373	15.027	45.976	19.156	1.00 16.66
ATOM	2859	С	ALA	373	15.024	46.018	16.665	1.00 18.79
ATOM	2860	0	ALA	373	15.301	45.004	16.018	1.00 20.02
ATOM	2861	N	HIS	374	14.037	46.841	16.316	1.00 19.22
ATOM ATOM	2862	CA	HIS	374	13.243	46.560	15.122	1.00 20.89
ATOM	2863 2864	CB	HIS	374 374	12.025	47.489	15.052	1.00 20.98
ATOM	2865	CD2	HIS	374	10.948	47.131	16.029	1.00 19.79
ATOM	2866	ND1	HIS	374	9.833	46.065 47.914	16.855 16.229	1.00 19.53
MOTA	2867	CE1	HIS	374	9.057	47.347	17.137	1.00 19.92
ATOM	2868		HIS	374	9.629	46.223	17.532	1.00 18.61
ATOM	2869	C	HIS	374	14.075	46.696	13.866	1.00 21.57
ATOM	2870	ō	HIS	374	14.136	45.789	13.058	1.00 21.42
ATOM	2871	N	MSE	375	14.722	47.835	13,698	1.00 24.00
MOTA	2872	CA	MSE	375	15.561	48.027	12,528	1.00 26.05
ATOM	2873	CB	MSE	375	16.390	49.311	12.666	1.00 28.31
MOTA	2874	CG	MSE	375	15.671	50.558	12.197	1.00 31.46
ATOM	2875	SE	MSE	375	15.246	50.448	10.400	1.00 41.26
MOTA	2876	CE	MSE	375	16.340	51.745	9.680	1.00 36.51
MOTA	2877	C	MSE	375	16.476	46.810	12.390	1.00 25.84
ATOM	2878	0	MSE	375	16.501	46.159	11.351	1.00 26.84
ATOM	2879	N	CYS	376	17.200	46.489	13.455	1.00 25.61
ATOM	2880	CA	CYS	376	18.107	45.349	13.436	1.00 25.11
ATOM	2881	CB	CYS	376	18.693	45.117	14.831	1.00 26.04
ATOM	2882	SG	CYS	376	20.038	43.879	14.876	1.00 27.98
ATOM	2883	С	CYS	376	17.445	44.058	12.931	1.00 24.01
ATOM ATOM	2884	O N	CYS	376	18.015	43.369	12.078	1.00 24.35
ATOM	2885 2886	CA	SER	377 377	16.251	43.741	13.443	1.00 22.14
ATOM	2000	CA	ack	3//	15.519	42.531	13.038	1.00 20.58

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ATOM 2887 CB SER 377 14.203 42.399 13.811 1.00 20.36 ATOM 2889 C SER 377 13.233 43.325 13.338 1.00 20.95 ATOM 2889 C SER 377 15.154 41.484 10.900 1.00 19.23 ATOM 2891 N ALA 378 14.995 43.715 10.980 1.00 19.23 ATOM 2891 N ALA 378 14.995 43.715 10.980 1.00 19.23 ATOM 2891 N ALA 378 14.995 43.715 10.980 1.00 19.23 ATOM 2892 CA ALA 378 14.723 43.787 9.549 1.00 19.32 ATOM 2895 C ALA 378 14.521 45.243 9.119 1.00 18.02 ATOM 2895 C ALA 378 15.958 43.186 8.874 1.00 19.32 ATOM 2895 C ALA 378 15.958 43.186 8.874 1.00 19.32 ATOM 2895 C ALA 378 15.958 43.186 8.874 1.00 19.32 ATOM 2897 C ALA 378 15.958 43.186 8.874 1.00 19.40 ATOM 2897 C ALA 378 15.958 43.186 8.874 1.00 19.40 ATOM 2897 C ALA 378 15.958 43.186 8.874 1.00 19.40 ATOM 2897 C ALA 378 15.860 42.200 8.093 1.00 18.55 ATOM 2897 C ALY 379 18.381 43.271 8.669 1.00 20.08 ATOM 2897 C ALY 379 18.547 41.752 8.754 1.00 20.07 ATOM 2897 C ALY 379 18.547 41.120 9.936 1.00 18.51 ATOM 2897 C ALY 379 18.547 41.123 7.704 1.00 20.07 ATOM 2900 N LEU 380 18.547 41.201 9.936 1.00 18.61 ATOM 2901 CA LEU 380 18.596 39.763 10.110 1.00 18.64 ATOM 2902 CB LEU 380 18.699 39.763 10.110 1.00 18.64 ATOM 2902 CB LEU 380 18.744 37.881 11.816 1.00 17.82 ATOM 2905 CD LEU 380 18.747 37.881 11.816 1.00 17.82 ATOM 2905 CD LEU 380 18.575 37.512 13.285 1.00 16.34 ATOM 2905 C LEU 380 18.575 37.512 13.285 1.00 16.34 ATOM 2905 C LEU 380 17.580 38.989 9.341 1.00 19.55 ATOM 2907 C LEU 380 17.580 38.989 9.341 1.00 19.55 ATOM 2907 C LEU 380 17.580 38.989 9.341 1.00 19.56 ATOM 2912 C ALA 381 15.341 39.61 39.327 8.759 1.00 16.34 ATOM 2912 C ALA 381 15.341 39.61 39.327 8.759 1.00 20.07 ATOM 2915 C ALA 381 15.341 39.61 39.327 8.759 1.00 20.07 ATOM 2916 C ALA 381 15.341 39.91 39.832 1.00 20.07 ATOM 2910 C ALA 381 15.341 39.91 39.832 1.00 20.07 ATOM 2911 C ALA 381 15.341 39.91 39.832 1.00 20.07 ATOM 2912 C ALA 381 15.341 39.91 39.832 1.00 20.07 ATOM 2912 C ALA 381 15.341 39.91 39.832 1.00 20.07 ATOM 2913 N ALY 382 183 19.07 38.34 4.950 1.00 21.05 ATOM 2912 C VAL 383 19.64 29.79 ATOM 2913 C ALA 381 15.341 39.91 39.8	r.	igur 4							
ATOM 2888 OG SER 377 13.233 43.255 13.338 1.00 20.95 ATOM 2890 C SER 377 15.210 42.555 11.542 1.00 20.95 ATOM 2891 N ALA 378 14.995 43.715 10.980 1.00 19.23 ATOM 2892 CA ALA 378 14.995 43.715 10.980 1.00 19.23 ATOM 2893 CB ALA 378 14.521 45.243 9.119 1.00 18.02 ATOM 2894 C ALA 378 14.521 45.243 9.119 1.00 18.02 ATOM 2895 N ALA 378 14.521 45.243 9.119 1.00 18.02 ATOM 2895 N ALA 378 15.968 42.230 8.093 1.00 19.40 ATOM 2895 N ALA 378 15.968 42.230 8.093 1.00 19.52 ATOM 2895 N GLY 379 18.381 43.271 8.669 1.00 20.18 ATOM 2897 C GLY 379 18.547 41.762 8.734 1.00 20.07 ATOM 2898 C GLY 379 18.547 41.762 8.734 1.00 20.07 ATOM 2890 N LEU 380 18.424 41.201 9.936 1.00 18.51 ATOM 2901 CA LEU 380 18.493 39.763 10.110 1.00 18.41 ATOM 2902 CB LEU 380 18.493 39.711 11.579 1.00 18.49 ATOM 2903 CG LEU 380 18.794 37.586 11.816 1.00 17.82 ATOM 2905 CD LEU 380 18.579 37.561 11.383 1.00 15.94 ATOM 2906 C LEU 380 18.579 37.561 11.383 1.00 15.94 ATOM 2907 C LEU 380 18.579 37.581 11.816 1.00 17.82 ATOM 2908 N ALA 381 16.544 39.407 39.21 10.91 39.57 ATOM 2909 C A LEU 380 18.579 37.831 8.892 1.00 20.77 ATOM 2907 C LEU 380 17.580 38.938 9.341 1.00 19.55 ATOM 2909 C A LEU 380 17.580 38.938 9.341 1.00 19.83 ATOM 2909 C A LEU 380 17.580 38.938 9.341 1.00 19.83 ATOM 2910 C A LEU 380 17.580 38.938 9.341 1.00 19.63 ATOM 2910 C A LEU 380 17.580 38.938 9.341 1.00 19.63 ATOM 2910 C C ALA 381 15.341 39.327 8.759 1.00 19.87 ATOM 2911 C A LEU 380 17.895 37.833 8.892 1.00 20.77 ATOM 2912 C C A LEU 380 17.895 37.833 8.892 1.00 20.77 ATOM 2913 N ALY 381 15.341 39.77 6.255 1.00 20.77 ATOM 2914 CA ALA 381 15.421 37.773 6.255 1.00 20.77 ATOM 2915 C GL VAL 381 15.421 37.773 6.255 1.00	* moss	2007	-	000	377				
ATOM 2889 C SER 377									
ATOM 2890 O SER 377									
ATOM 2891 N ALA 378 14.995 43.715 10.980 1.00 19.64 ATOM 2892 CA ALA 378 14.525 45.243 9.119 1.00 18.02 ATOM 2893 CB ALA 378 14.521 45.243 9.119 1.00 18.02 ATOM 2895 N ALA 378 15.958 43.186 8.874 1.00 19.02 ATOM 2895 N ALA 378 15.958 43.186 8.874 1.00 19.02 ATOM 2895 N ALA 378 15.860 42.230 8.093 1.00 18.65 ATOM 2895 N ALA 378 15.860 42.230 8.093 1.00 18.55 ATOM 2897 CA GLY 379 18.587 41.762 8.734 1.00 20.18 ATOM 2899 O GLY 379 18.587 41.762 8.734 1.00 19.52 ATOM 2899 O GLY 379 18.597 41.13 7.704 1.00 20.07 ATOM 2901 CA LEU 380 18.492 41.201 9.936 1.00 18.44 ATOM 2901 CA LEU 380 18.499 39.371 11.579 1.00 18.49 ATOM 2901 CA LEU 380 18.499 39.371 11.579 1.00 18.49 ATOM 2902 CB LEU 380 18.499 39.371 11.579 1.00 18.49 ATOM 2905 CD2 LEU 380 18.499 39.371 11.579 1.00 18.49 ATOM 2905 CD2 LEU 380 18.499 39.371 11.579 1.00 18.49 ATOM 2905 CD2 LEU 380 18.596 39.783 11.00 16.94 ATOM 2907 O LEU 380 18.557 37.586 11.383 1.00 16.94 ATOM 2907 O LEU 380 17.580 38.938 9.341 1.00 19.55 ATOM 2907 O LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2907 O LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2907 O LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2901 CB ALA 381 15.331 38.713 8.713 8.713 8.713 ATOM 2901 CB ALA 381 15.331 38.713 8.752 10.00 19.87 ATOM 2901 CB ALA 381 15.331 38.713 8.752 10.00 19.87 ATOM 2910 CB ALA 381 15.331 38.713 8.752 10.00 19.87 ATOM 2910 CB ALA 381 15.331 38.713 8.753 10.00 19.67 ATOM 2911 C ALA 381 15.531 38.713 8.753 10.00 20.07 ATOM 2911 C ALA 381 15.531 38.713 8.753 10.00 20.07 ATOM 2911 C ALA 381 15.621 37.73 6.669 1.00 20.10 ATOM 2914 CA GLY 382 17.670 38.954 4.903 1.00 21.05 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 21.05 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 22.07 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 22.07 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 22.07 ATOM 2917 N VAL 383 19.979 36.614 4.655 1.00 22.07 ATOM 2917 N VAL 383 19.979 36.614 4.903 1.00 22.07 ATOM 2917 N VAL 383 19.999 36.6196 1.00 21.05 ATOM 2918 C GLY 384 184 185 185 185 185 185 185 185 185 185 185									
ATOM 2892 CA ALA 378 14.723 43.767 9.549 1.00 19.30 ATOM 2894 C ALA 378 14.521 45.243 9.119 1.00 18.00 ATOM 2895 CO ALA 378 15.958 43.186 8.874 1.00 19.40 ATOM 2895 CO ALA 378 15.958 43.186 8.874 1.00 19.40 ATOM 2897 CA GLY 379 18.381 43.740 9.222 1.00 20.18 ATOM 2897 CA GLY 379 18.381 43.741 9.222 1.00 20.18 ATOM 2897 CA GLY 379 18.381 43.271 8.669 1.00 20.18 ATOM 2898 C GLY 379 18.547 41.152 7.704 1.00 20.07 ATOM 2890 O GLY 379 18.544 41.113 7.704 1.00 20.07 ATOM 2890 O GLY 379 18.544 41.113 7.704 1.00 20.07 ATOM 2890 C GLY 379 18.544 41.113 7.704 1.00 20.07 ATOM 2900 C B LEU 380 18.596 39.763 10.110 10.18.49 ATOM 2901 CA LEU 380 18.596 39.763 10.110 10.18.49 ATOM 2904 CD1 LEU 380 18.744 37.881 11.816 1.00 17.82 ATOM 2905 CD2 LEU 380 18.744 37.881 11.816 1.00 17.82 ATOM 2905 CD2 LEU 380 18.597 37.512 13.285 1.00 16.34 ATOM 2905 C LEU 380 18.597 37.512 13.285 1.00 16.34 ATOM 2905 C LEU 380 18.597 37.512 13.285 1.00 16.34 ATOM 2905 C LEU 380 17.895 37.833 8.892 1.00 20.67 ATOM 2907 C LEU 380 17.895 37.833 8.892 1.00 20.67 ATOM 2907 C LEU 380 17.895 37.833 8.892 1.00 20.67 ATOM 2907 C LEU 380 17.895 37.833 8.892 1.00 20.67 ATOM 2907 C LEU 380 17.895 37.833 8.892 1.00 20.67 ATOM 2907 C LEU 380 17.895 37.833 8.892 1.00 20.67 ATOM 2907 C ALA 381 15.311 38.713 8.496 1.00 20.17 ATOM 2907 C ALA 381 15.313 38.713 8.496 1.00 20.17 ATOM 2907 C ALA 381 15.541 37.773 6.297 1.00 19.87 ATOM 2910 CB ALA 381 15.541 37.773 6.297 1.00 19.87 ATOM 2911 C ALA 381 15.541 37.773 6.297 1.00 21.05 ATOM 2912 C ALA 381 15.541 37.773 6.297 1.00 21.05 ATOM 2912 C ALA 381 15.541 37.773 6.297 1.00 21.05 ATOM 2914 C ALG UN 382 11.6414 39.874 49.931 1.00 21.05 ATOM 2915 C GLY 382 383 18.547 7.099 1.00 21.05 ATOM 2916 C ALA 381 18.541 37.773 6.297 1.00 21.05 ATOM 2912 C ALA 381 18.541 37.773 6.297 1.00 21.05 ATOM 2912 C ALA 381 18.541 37.773 6.297 1.00 21.05 ATOM 2912 C ALA 381 383 18.542 37.828 5.695 1.00 21.05 ATOM 2916 C ALA 381 383 18.541 37.773 6.297 1.00 21.05 ATOM 2918 C AVAL 383 18.579 38.787 8.585 1.00 21.03 3.70 ATOM 2912 C ALA 381 38									
ATOM 2893 CB ALA 378							43.715	10.980	1.00 19.64
ATOM							43.787	9.549	
ATOM								9.119	1.00 18.02
ATOM 2896 N GLY 379 17.123 43.740 9.222 1.00 20.16 ATOM 2897 CA GLY 379 18.587 41.762 8.734 1.00 19.52 ATOM 2898 C GLY 379 18.587 41.762 8.734 1.00 19.52 ATOM 2900 N LEU 380 18.754 41.113 7.704 1.00 20.07 ATOM 2901 CA LEU 380 18.596 39.763 10.110 1.00 18.91 ATOM 2902 CB LEU 380 18.596 39.763 10.110 1.00 18.91 ATOM 2902 CB LEU 380 18.744 37.881 11.816 1.00 17.82 ATOM 2904 CD1 LEU 380 18.774 37.881 11.816 1.00 17.82 ATOM 2905 CD2 LEU 380 18.597 37.512 13.285 1.00 16.94 ATOM 2906 C LEU 380 18.597 37.512 13.285 1.00 16.94 ATOM 2907 CD LEU 380 18.597 37.512 13.285 1.00 16.94 ATOM 2908 N ALA 381 16.534 39.447 9.211 1.00 19.83 ATOM 2909 CA ALA 381 15.311 38.713 8.892 1.00 20.67 ATOM 2907 CB ALA 381 15.311 38.713 8.496 1.00 20.17 ATOM 2910 CB ALA 381 15.5311 38.713 8.496 1.00 20.17 ATOM 2911 C ALA 381 15.634 39.747 9.211 1.00 19.87 ATOM 2912 C ALA 381 15.634 39.773 6.525 10.00 21.05 ATOM 2914 CA GLY 382 16.574 39.874 6.567 1.00 21.05 ATOM 2915 C GLY 382 16.561 39.954 4.903 1.00 21.05 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 21.05 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 21.05 ATOM 2916 C GLY 382 17.670 38.954 4.903 1.00 21.05 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 21.05 ATOM 2915 C GLY 382 17.708 38.719 5.555 1.00 22.33 ATOM 2915 C GLY 382 17.708 38.719 5.555 1.00 22.33 ATOM 2915 C GLY 382 17.708 38.719 3.832 1.00 23.74 ATOM 2915 C GLY 382 17.708 38.719 3.832 1.00 23.74 ATOM 2915 C GLY 382 17.708 38.719 3.832 1.00 23.74 ATOM 2915 C GLY 382 17.708 38.719 3.832 1.00 23.74 ATOM 2915 C GLY 383 13.542 37.728 5.655 1.00 21.03 ATOM 2915 C GLY 382 31.747 38.778 5.656 1.00 22.33 ATOM 2917 N VAL 383 18.579 38.778 5.855 1.00 22.83 ATOM 2918 C GLY AL 383 18.579 38.778 5.855 1.00 22.83 ATOM 2919 C B ALA 381 15.541 37.708 5.661 1.00 22.80 ATOM 2915 C GLY 382 38.544 5.691 1.00 22.80 ATOM 2917 N VAL 383 19.775 36.423 5.691 1.00 22.92 ATOM 2918 C GLY AL 383 19.775 36.423 5.691 1.00 22.92 ATOM 2919 C GLY AL 383 19.775 36.423 5.691 1.00 22.92 ATOM 2919 C GLY AL 383 19.775 36.423 5.691 1.00 22.92 ATOM 2910 C GLY AL 383 19.77	ATOM	2894	C	ALA	378	15.958	43.186	8.874	1.00 19.40
ATOM 2897 CA GLY 379 18.581 43.271 8.669 1.00 20.05 ATOM 2898 C GLY 379 18.547 41.762 8.734 1.00 19.55 ATOM 2890 N LEU 380 18.442 41.201 9.936 1.00 19.55 ATOM 2901 CA LEU 380 18.492 41.201 9.936 1.00 18.61 ATOM 2902 CB LEU 380 18.499 39.371 11.579 1.00 18.64 ATOM 2903 CG LEU 380 18.499 39.371 11.579 1.00 18.49 ATOM 2904 CD1 LEU 380 20.215 37.586 11.383 1.00 16.94 ATOM 2905 CD2 LEU 380 18.574 37.581 11.816 1.00 17.82 ATOM 2906 C LEU 380 18.574 37.581 11.816 1.00 17.82 ATOM 2907 C LEU 380 18.575 37.512 13.285 1.00 16.94 ATOM 2908 N ALA 381 15.593 39.389 9.341 1.00 19.56 ATOM 2909 CA ALA 381 15.513 38.713 8.496 1.00 20.67 ATOM 2909 CA ALA 381 15.513 38.713 8.496 1.00 20.77 ATOM 2910 CB ALA 381 15.513 38.713 8.496 1.00 20.17 ATOM 2911 C ALA 381 15.618 38.744 7.009 1.00 21.05 ATOM 2912 C ALA 381 15.413 37.773 6.269 1.00 21.05 ATOM 2913 N GLY 382 16.574 37.773 6.269 1.00 21.05 ATOM 2914 CA GLY 382 16.576 37.775 6.567 1.00 22.63 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 23.14 ATOM 2916 O GLY 382 17.708 38.319 38.32 1.00 23.14 ATOM 2917 C ALA 381 15.41 37.773 6.269 1.00 21.05 ATOM 2918 N VAL 383 18.579 37.785 5.859 1.00 12.05 ATOM 2918 C A VAL 383 18.579 38.778 5.859 1.00 21.05 ATOM 2919 CB VAL 383 18.579 38.778 5.859 1.00 21.05 ATOM 2914 CA GLY 382 17.670 38.954 4.903 1.00 23.14 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 23.14 ATOM 2916 O GLY 382 17.708 38.319 3.832 1.00 23.14 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.04 ATOM 2918 CA VAL 383 18.579 38.778 5.859 1.00 21.05 ATOM 2919 CB VAL 383 19.599 35.681 4.675 1.00 22.67 ATOM 2917 C GLY 382 31.709 38.319 3.832 1.00 23.74 ATOM 2918 CA VAL 383 19.599 35.681 4.675 1.00 22.67 ATOM 2919 CB VAL 383 19.999 35.681 4.675 1.00 23.52 ATOM 2919 CB VAL 383 19.999 35.681 4.675 1.00 23.52 ATOM 2917 CG LY 384 11.384 11.394 31.594 37.782 5.859 1.00 23.05 ATOM 2918 CA VAL 383 19.999 35.681 4.675 1.00 23.65 ATOM 2929 CG VAL 383 19.999 35.681 4.675 1.00 23.65 ATOM 2930 C VAL 383 19.999 35.681 4.675 1.00 23.65 ATOM 2931 C TLE 384 16.910 34.721 5.820 1.00 24.54 ATOM 2931 C TLE	MOTA	2895	0	ALA	378	15.860	42.230	8.093	1.00 18.55
ATOM 2898 C GLY 379 18.547 41.762 8.734 1.00 19.50 ATOM 2890 N LEU 380 18.492 41.201 9.936 1.00 18.61 ATOM 2900 N LEU 380 18.492 41.201 9.936 1.00 18.61 ATOM 2901 CA LEU 380 18.492 41.201 9.936 1.00 18.49 ATOM 2902 CB LEU 380 18.493 93.371 11.579 1.00 18.49 ATOM 2903 CD LEU 380 18.493 93.371 11.579 1.00 18.49 ATOM 2904 CD LEU 380 18.493 93.371 11.579 1.00 18.49 ATOM 2905 CD LEU 380 18.596 39.765 10.110 1.00 17.82 ATOM 2905 CD LEU 380 18.597 37.512 13.285 1.00 16.94 ATOM 2905 CD LEU 380 18.597 37.512 13.285 1.00 16.94 ATOM 2905 CD LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2907 C LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2907 C LEU 380 17.580 38.939 9.341 1.00 19.56 ATOM 2907 C LEU 380 17.580 38.939 9.341 1.00 19.56 ATOM 2907 C A ALA 381 15.311 38.713 8.496 1.00 20.67 ATOM 2910 CB ALA 381 15.311 38.713 8.496 1.00 20.17 ATOM 2910 CB ALA 381 15.531 38.713 8.496 1.00 20.17 ATOM 2911 C ALA 381 15.638 38.746 7.009 1.00 21.05 ATOM 2912 C ALA 381 15.638 38.746 7.009 1.00 21.05 ATOM 2913 N GLY 382 16.574 39.874 9.55 7.75 1.00 22.53 ATOM 2914 CA GLY 382 16.591 39.955 5.175 1.00 22.53 ATOM 2915 C GLY 382 17.600 38.954 4.903 1.00 23.10 ATOM 2915 C GLY 382 17.708 39.955 5.175 1.00 23.14 ATOM 2916 C GLY 382 17.708 39.955 5.155 1.00 23.14 ATOM 2916 C GLY AL 383 18.579 38.778 5.859 1.00 23.14 ATOM 2916 C GLY AL 383 19.575 36.423 5.615 1.00 23.14 ATOM 2917 N VAL 383 19.575 36.423 5.615 1.00 23.14 ATOM 2917 C GLY AL 383 19.575 36.423 5.615 1.00 23.14 ATOM 2917 N VAL 383 19.575 36.423 5.615 1.00 23.14 ATOM 2917 C GLY AL 383 19.575 36.423 5.615 1.00 23.24 ATOM 2925 C GLY AL 383 19.075 36.423 5.615 1.00 23.57 ATOM 2927 C GLY AL 383 19.075 36.423 5.615 1.00 23.57 ATOM 2927 C GLY AL 383 19.075 36.423 5.615 1.00 23.57 ATOM 2927 C GLY AL 383 19.075 36.423 5.615 1.00 23.57 ATOM 2927 C GLY AL 383 19.075 36.423 5.615 1.00 23.57 ATOM 2927 C GLY AL 383 19.075 36.423 5.615 1.00 23.57 ATOM 2927 C GLY AL 383 19.075 36.423 5.615 1.00 23.57 ATOM 2927 C GLY AL 383 19.075 36.423 5.615 1.00 23.57 ATOM 2927 C GLY AL 383 19.075 36.423 5.615 1.00 2	MOTA	2896	N	GLY	379	17.123	43.740	9.222	1.00 20.18
ATOM 2999 O GLY 379 18.754 41.113 7.704 1.00 20.07 ATOM 2901 CA LEU 380 18.424 41.201 9.936 1.00 18.474 ATOM 2902 CB LEU 380 18.596 39.763 10.110 1.00 18.74 ATOM 2902 CB LEU 380 18.489 39.371 11.579 1.00 18.49 ATOM 2903 CG LEU 380 18.489 39.371 11.579 1.00 18.49 ATOM 2904 CD1 LEU 380 20.215 37.586 11.383 1.00 16.94 ATOM 2905 CD2 LEU 380 18.557 37.586 11.383 1.00 16.94 ATOM 2906 C LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2906 C LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2906 C LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2907 O LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2907 C LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2907 C LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2908 N ALA 381 15.351 38.713 8.496 1.00 20.67 ATOM 2910 CB ALA 381 15.311 38.713 8.496 1.00 20.17 ATOM 2910 CB ALA 381 15.513 13.713 8.496 1.00 20.17 ATOM 2911 C ALA 381 15.638 38.746 7.000 19.87 ATOM 2912 C ALA 381 15.638 38.746 7.000 10.0 21.06 ATOM 2912 C ALA 381 15.638 38.746 7.000 10.0 21.05 ATOM 2913 N GLY 382 16.514 39.955 51.75 1.00 22.63 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 21.03 ATOM 2916 C GLY 382 17.670 38.954 4.903 1.00 21.03 ATOM 2916 C GLY 382 17.670 38.954 4.903 1.00 23.10 ATOM 2917 C ALA 381 18.579 38.778 5.859 1.00 22.63 ATOM 2917 C ALA 381 18.579 38.778 5.859 1.00 22.63 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 22.63 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.174 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.174 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.174 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.174 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.574 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.574 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.574 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.575 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.575 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.575 ATOM 2917 C ALA 383 18.579 38.778 5.859 1.00 23.575 ATOM 2917 C ALA 383 18.579 38.778 5.861 1.00 23.68 ATOM 2918 C ALA 383 38.58 38.58 38.58 38.59 39.98 1.00 23.575 ATOM 2918 C ALA 383 38.5	ATOM	2897	CA	GLY	379	18.381	43.271	8.669	1.00 20.06
ATOM 2899 O GLY 379 18.754 41.113 7.704 1.00 20.07 ATOM 2901 CA LEU 380 18.424 41.201 9.936 1.00 18.61 ATOM 2901 CA LEU 380 18.596 39.765 10.110 1.00 18.49 ATOM 2903 CB LEU 380 18.794 37.881 11.816 1.00 17.82 ATOM 2903 CG LEU 380 18.774 37.881 11.816 1.00 17.82 ATOM 2905 CD 2.250 380 18.757 37.881 11.816 1.00 17.82 ATOM 2905 CD 2.250 380 18.757 37.881 11.816 1.00 17.82 ATOM 2905 CD 2.250 380 18.557 37.586 11.383 1.00 16.94 ATOM 2905 CD 2.250 380 18.557 37.586 11.383 1.00 16.94 ATOM 2906 C LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2906 C LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2908 N ALA 381 16.354 39.447 9.211 1.00 19.83 ATOM 2907 CA ALA 381 15.311 38.713 8.466 1.00 20.67 ATOM 2910 CB ALA 381 15.513 13.713 8.466 1.00 20.17 ATOM 2910 CB ALA 381 15.638 38.746 7.000 19.07 10.00 19.87 ATOM 2911 C ALA 381 15.638 38.746 7.000 19.07 10.00 19.87 ATOM 2912 C ALA 381 15.638 38.746 7.000 10.00 21.07 ATOM 2915 C GLY 382 17.670 38.956 5.175 1.00 21.03 ATOM 2915 C GLY 382 17.670 38.956 5.175 1.00 21.03 ATOM 2915 C GLY 382 17.670 38.956 5.175 1.00 23.10 ATOM 2916 C GLY 382 17.670 38.956 5.175 1.00 23.14 ATOM 2916 C GLY 382 17.670 38.956 5.175 1.00 23.14 ATOM 2917 C ALA 381 18.579 38.778 5.859 1.00 21.03 ATOM 2918 C ALA 381 381 5.420 37.828 5.859 1.00 21.03 ATOM 2918 C ALA 383 18.579 38.778 5.859 1.00 21.33 ATOM 2918 CA VAL 383 18.579 38.778 5.859 1.00 21.33 ATOM 2918 CA VAL 383 19.599 38.778 6.614 1.00 22.47 ATOM 2917 C ALA 383 19.599 38.778 6.643 1.00 22.87 ATOM 2917 C ALA 383 19.999 35.681 4.675 1.00 22.47 ATOM 2917 C ALA 383 19.999 35.681 4.675 1.00 22.87 ATOM 2917 C ALA 383 19.999 35.681 4.675 1.00 22.87 ATOM 2917 C ALA 383 19.999 35.681 4.675 1.00 22.87 ATOM 2917 C ALA 383 19.999 35.681 4.675 1.00 22.80 ATOM 2917 C ALA 383 19.999 35.681 4.675 1.00 22.80 ATOM 2918 C ALA 383 19.999 35.681 4.675 1.00 22.80 ATOM 2918 C ALA 383 19.999 35.681 4.675 1.00 22.80 ATOM 2918 C ALA 383 19.999 35.681 4.675 1.00 22.80 ATOM 2918 C ALA 383 19.999 35.681 4.675 1.00 22.80 ATOM 2918 C ALA 384 11.00 38.81 11.00 28.98 ATOM 2918 C ALA 38	MOTA	2898	C	GLY	379	18.547	41.762	8.734	1.00 19.52
ATOM	MOTA	2899	0	GLY	379	18.754		7.704	1.00 20.07
ATOM 2901 CA LEU 380 18.596 39.763 10.110 1.00 18.49 ATOM 2903 CG LEU 380 18.489 39.763 10.110 1.00 18.49 ATOM 2904 CD1 LEU 380 20.215 37.586 11.381 1.00 16.34 ATOM 2905 CD2 LEU 380 18.774 37.881 11.816 1.00 17.82 ATOM 2906 C LEU 380 18.575 37.512 13.285 1.00 16.34 ATOM 2907 C LEU 380 18.557 37.512 13.285 1.00 16.34 ATOM 2907 C LEU 380 17.580 38.389 9.341 1.00 19.56 ATOM 2908 N ALA 381 16.354 39.447 9.211 1.00 19.87 ATOM 2909 CA ALA 381 15.311 38.713 8.496 1.00 20.67 ATOM 2910 CB ALA 381 15.311 39.13 8.496 1.00 20.17 ATOM 2911 C ALA 381 15.311 39.13 8.713 8.496 1.00 20.17 ATOM 2912 C ALA 381 15.421 37.773 6.269 1.00 21.06 ATOM 2915 C ALA 381 15.421 37.773 6.269 1.00 21.06 ATOM 2912 O ALA 381 15.421 37.773 6.269 1.00 21.05 ATOM 2913 N GLY 382 16.561 39.965 5.175 1.00 21.33 ATOM 2913 C ALA 381 15.421 37.773 6.269 1.00 21.33 ATOM 2914 CA GLY 382 17.708 39.319 3.832 1.00 22.50 ATOM 2919 C A VAL 383 19.642 37.828 5.615 1.00 22.13 ATOM 2919 C A VAL 383 19.642 37.828 5.615 1.00 22.13 ATOM 2919 C A VAL 383 19.642 37.828 5.615 1.00 22.13 ATOM 2912 C GU VAL 383 19.642 37.828 5.615 1.00 22.80 ATOM 2922 C VAL 383 19.075 36.423 5.619 1.00 21.83 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.80 ATOM 2925 C GI VAL 383 19.075 36.423 5.639 1.00 22.81 ATOM 2927 CG2 VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG2 VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG2 VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG2 VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG2 LEU 384 17.124 34.551 8.179 1.00 24.54 ATOM 2927 CG2 LEU 384 17.124 34.551 8.179 1.00 24.54 ATOM 2927 CG2 LEU 384 17.124 34.551 8.179 1.00 24.54 ATOM 2929 CH LEU 384 17.243 34.551 8.179 1.00 24.54 ATOM 2930 C ALB 384 17.124 34.551 8.179 1.00 24.54 ATOM 2931 N ALB 384 15.19.93 36.841 1.00 27.99 ATOM 2932 C ALB 384 15.19.93 36.841 1.00 27.99 ATOM 2932 C ALB 384 15.19.93 36.84 1.00 27.99 ATOM 2934 C ALB 384 15.19.93 36.84 1.00 27.99 ATOM 2935 C ALB 384 16.910 34.344 5.561 1.00 24.54 ATOM 2936 C ALB 384 16.910 34.344 5.561 1.00 24.57 ATOM 2937 C ALB 384 16.910 34	MOTA	2900	N	LEU	380	18.442	41.201	9.936	1.00 18.61
ATOM 2902 CB LEU 380	MOTA	2901	CA	LEU	380	18.596			
ATOM 2903 CG LEU 380 18.774 37.881 11.816 1.00 17.89 ATOM 2905 CD2 LEU 380 20.215 37.586 11.383 1.00 16.94 ATOM 2905 CD2 LEU 380 18.557 37.512 13.285 1.00 16.34 ATOM 2907 C LEU 380 17.895 37.831 8.892 1.00 20.67 ATOM 2907 C LEU 380 17.895 37.833 8.892 1.00 20.67 ATOM 2909 CA ALA 381 16.554 39.447 9.211 1.00 19.83 ATOM 2909 CA ALA 381 15.311 39.13 8.496 1.00 20.17 ATOM 2910 CB ALA 381 15.311 39.13 8.713 8.496 1.00 20.17 ATOM 2911 C ALA 381 15.511 39.13 8.713 8.496 1.00 20.17 ATOM 2912 C ALA 381 15.541 39.476 7.009 1.00 21.06 ATOM 2912 C ALA 381 15.421 37.773 6.269 1.00 21.06 ATOM 2913 N GLY 382 16.561 39.965 5.175 1.00 21.05 ATOM 2913 N GLY 382 16.561 39.965 5.175 1.00 21.33 ATOM 2915 C GLY 382 17.708 39.319 3.832 1.00 23.10 ATOM 2916 C GLY 382 17.708 39.319 3.832 1.00 23.10 ATOM 2917 N VAL 383 18.579 38.778 5.859 1.00 21.83 ATOM 2919 CB VAL 383 19.642 37.828 5.615 1.00 22.80 ATOM 2920 CGI VAL 383 19.642 37.828 5.615 1.00 22.80 ATOM 2922 C VAL 383 19.075 36.423 5.619 1.00 21.85 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.80 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.80 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2925 CA LEE 384 17.124 34.551 8.179 1.00 24.54 ATOM 2925 CA LE 384 17.124 34.551 8.179 1.00 24.54 ATOM 2925 CA LE 384 17.124 34.551 8.179 1.00 24.54 ATOM 2925 CA LE 384 17.124 34.551 8.179 1.00 24.57 ATOM 2935 CA LE 384 17.124 34.551 8.179 1.00 24.59 ATOM 2935 CA LE 384 17.124 34.551 8.179 1.00 24.59 ATOM 2935 CA LE 384 17.124 34.551 8.179 1.00 24.59 ATOM 2935 CA LE 384 17.124 34.551 8.179 1.00 24.59 ATOM 2935 CA AND 385 11.586 35.479 2.918 1.00 25.92 ATOM 2938 C AND 385 11.586 35.479 2.918 1.00 25.92 ATOM 2938 C AND 385 11.586 35.479 2.918 1.00 25.92 ATOM 2938 C AND 385 11.586 35.47	MOTA	2902	CB	LEU	380	18.489		11.579	
ATOM 2904 CD1 LEU 380 20.215 37.586 11.383 1.00 16.34 ATOM 2905 CD2 LEU 380 18.557 37.586 11.383 1.00 16.34 ATOM 2906 C LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2907 O LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2908 N ALA 381 16.354 39.447 9.211 1.00 19.56 ATOM 2910 CB ALA 381 15.311 38.713 8.496 1.00 20.67 ATOM 2910 CB ALA 381 15.311 38.713 8.496 1.00 20.17 ATOM 2911 C ALA 381 15.638 38.746 7.009 1.00 21.05 ATOM 2912 O ALA 381 15.638 38.746 7.009 1.00 21.05 ATOM 2914 CA GLY 382 16.541 39.955 5.157 1.00 22.03 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 23.10 ATOM 2915 C GLY 382 17.670 38.954 4.903 1.00 23.14 ATOM 2917 N VAL 383 18.579 38.778 5.859 1.00 23.14 ATOM 2919 CB VAL 383 18.579 38.778 5.859 1.00 23.14 ATOM 2919 CB VAL 383 18.579 38.778 5.859 1.00 23.14 ATOM 2910 CG1 VAL 383 19.642 37.828 5.651 5.00 22.37 ATOM 2912 C VAL 383 19.642 37.828 5.651 5.00 22.37 ATOM 2912 C VAL 383 19.505 5.639 1.00 21.35 ATOM 2921 CG2 VAL 383 19.505 5.639 1.00 22.37 ATOM 2921 CG2 VAL 383 19.49 35.681 4.675 1.00 22.37 ATOM 2922 C VAL 383 19.795 36.423 5.639 1.00 22.32 ATOM 2923 CG VAL 383 19.795 36.423 5.639 1.00 22.32 ATOM 2924 N ILE 384 19.795 36.423 5.639 1.00 22.52 ATOM 2925 CA ILE 384 19.795 36.423 5.639 1.00 22.52 ATOM 2925 CA ILE 384 19.795 36.423 5.639 1.00 22.55 ATOM 2925 CA ILE 384 19.475 38.681 4.675 1.00 23.52 ATOM 2925 CA ILE 384 19.475 38.681 4.675 1.00 23.52 ATOM 2925 CA ILE 384 19.124 34.551 8.179 1.00 23.52 ATOM 2925 CA ILE 384 19.124 34.551 8.179 1.00 23.52 ATOM 2925 CA ILE 384 19.124 34.551 8.179 1.00 23.65 ATOM 2931 C ILE 384 19.124 34.551 8.179 1.00 23.65 ATOM 2931 C ILE 384 19.124 34.551 8.179 1.00 23.65 ATOM 2931 C ILE 384 19.124 34.551 8.179 1.00 23.65 ATOM 2931 C ILE 384 19.127 34.861 10.661 1.00 23.69 ATOM 2931 C ILE 384 19.127 34.861 10.661 1.00 23.69 ATOM 2931 C ILE 384 19.127 34.861 10.661 1.00 23.69 ATOM 2931 C ILE 384 19.127 34.861 10.661 1.00 23.69 ATOM 2931 C ILE 384 19.127 34.861 10.661 1.00 23.69 ATOM 2931 C ILE 384 19.127 34.921 5.820 1.00 23.69 ATOM 2931 C ILE 384 19.127 34.861 10.661 1	MOTA	2903	CG	LEU	380	18.774			
ATOM 2905 CD2 LBU 380	MOTA	2904	CD1	LEU	380				
ATOM 2906 C LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2907 O LEU 380 17.580 38.938 9.341 1.00 19.56 ATOM 2908 N ALA 381 16.354 39.447 9.211 1.00 19.83 ATOM 2910 CB ALA 381 15.311 38.713 8.496 1.00 20.21 38.71 ATOM 2910 CB ALA 381 15.311 38.713 8.496 1.00 21.95 ATOM 2912 CA ALA 381 15.431 39.247 8.759 1.00 21.95 ATOM 2914 CA ALY 382 16.541 39.773 6.269 1.00 21.05 ATOM 2914 CA GLY 382 17.670 38.954 4.903 1.00 22.13 ATOM 2916 O GLY									
ATOM 2907 O LEU 380 17.895 37.833 8.892 1.00 20.87 ATOM 2908 N ALA 381 16.354 39.447 9.211 1.00 19.87 ATOM 2909 CA ALA 381 15.311 38.713 8.496 1.00 20.17 ATOM 2910 CB ALA 381 15.311 38.713 8.496 1.00 20.17 ATOM 2911 C ALA 381 15.961 39.327 8.759 1.00 19.87 ATOM 2912 O ALA 381 15.621 37.773 6.269 1.00 21.05 ATOM 2913 N GLY 382 16.174 39.874 6.567 1.00 21.05 ATOM 2913 N GLY 382 16.561 39.965 5.175 1.00 21.33 ATOM 2916 C GLY 382 17.760 38.974 6.567 1.00 21.33 ATOM 2917 N VAL 383 18.579 38.778 5.859 1.00 22.63 ATOM 2918 CA VAL 383 19.642 37.828 5.615 1.00 22.43 ATOM 2919 CB VAL 383 19.642 37.828 5.615 1.00 22.43 ATOM 2912 CC VAL 383 21.737 36.777 6.525 1.00 22.83 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.83 ATOM 2922 C VAL 383 19.075 36.423 5.639 1.00 22.83 ATOM 2925 CA LE 384 17.124 34.551 8.779 38.70 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2927 CG VAL 383 19.075 36.423 5.639 1.00 22.85 ATOM 2929 CA LE 384 17.124 34.551 8.179 1.00 24.174 ATOM 2927 CG LTE 384 16.533 33.143 8.283 1.00 22.50 ATOM 2930 C LE 384 16.910 34.324 5.561 1.00 23.59 ATOM 2931 O TLE 384 17.124 34.551 8.179 1.00 24.79 ATOM 2931 O TLE 384 17.124 34.551 8.179 1.00 24.79 ATOM 2932 N ASN 385 15.874 35.486 10.00 23.69 ATOM 2934 N ASN 385 15.874 37.485 1.00 24.64 ATOM 2934 CA ASN 385 15.874 37.485 1.00 24.69 ATOM 2934 CA ASN 385 15.874 37.975 5.484 1.00 25.98 ATOM 2937 ND ASN 385 15.874 37.975 5.484 1.00 25.98 ATOM 2937 ND ASN 385 15.874 37.975 5.484 1.00 25.98 ATOM 2937 ND ASN 385 15.874 37.975 5.484 1.00									
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ATOM 2942 CB ARG 386 18.840 35.261 1.446 1.00 32.62 ATOM 2943 CG ARG 386 19.697 36.147 0.214 1.00 33.28 ATOM 2944 CD ARG 386 20.908 37.059 0.284 1.00 34.52									
ATOM 2943 CG ARG 386 19.697 36.147 0.214 1.00 33.28 ATOM 2944 CD ARG 386 20.908 37.059 0.284 1.00 34.52									
ATOM 2944 CD ARG 386 20.908 37.059 0.284 1.00 34.52									
ATOM 2945 NE ARG 386 21.923 36.698 -0.704 1.00 35.29									
	ATOM	2945	NE	ARG	386	21.923	36.698	-0.704	1.00 35.29

Figur 4

MOTA	2946	CZ	ARG	386	21.812	36.910	-2.014	1.00 36.32
ATOM	2947	NH1		386	20.729	37.492	-2.518	1.00 35.95
ATOM	2948	NH2		386	22.782	36.525	-2.832	1.00 37.07
ATOM	2949	C	ARG	386	18.178	33.875	1.362	1.00 34.69
ATOM	2950	ō	ARG	386	18.077	33.232	0.320	1.00 35.70
ATOM	2951	N	MSE	387	18.710	33.383	2.480	1.00 35.70
ATOM	2952	CA	MSE	387	19.250	32.036	2.560	1.00 37.39
ATOM	2953	CB	MSE	387	19.903	31.828		1.00 37.39
ATOM	2954	CG	MSE	387	21.099		3.927	1.00 39.76
ATOM	2955	SE	MSE	387	21.099	32.754	4.186	
ATOM	2956	CE	MSE	387	21.738	32.552	5.859	
	2956	CE	MSE	387	18.179	30.694	6.097	1.00 44.67
ATOM				387		30.976	2.311	1.00 38.50
ATOM	2958	0	MSE		18.463	29.927	1.721	1.00 37.80
ATOM	2959	N	ARG	388	16.954	31.255	2.769	1.00 40.15
ATOM	2960	CA	ARG	388	15.808	30.352	2.586	1.00 41.28
ATOM	2961	CB	ARG	388	14.554	30.941	3.245	1.00 42.50
ATOM	2962	CG	ARG	388	13.268	30.115	3.069	1.00 42.73
ATOM	2963	CD	ARG	388	12.266	30.443	4.178	1.00 43.15
ATOM	2964	NE	ARG	388	10.965	29.787	4.012	1.00 44.47
ATOM	2965	CZ	ARG	388	10.049	30.134	3.104	1.00 44.46
ATOM	2966	NH1	ARG	388	10.283	31.139	2.269	1.00 44.11
ATOM	2967	NH2		388	8.895	29.478	3.033	1.00 44.15
ATOM .	2968	C	ARG	388	15.579	30.210	1.094	1.00 41.39
MOTA	2969	0	ARG	388	15.516	29.104	0.554	1.00 40.76
MOTA	2970	N	GLU	389	15.460	31.355	0.439	1.00 41.88
MOTA	2971	CA	GLU	389	15.275	31.405	-0.997	1.00 43.37
MOTA	2972	CB	GLU	389	15.211	32.867	-1.448	1.00 45.21
MOTA	2973	CG	GLU	389	15.227	33.079	-2.957	1.00 48.22
MOTA	2974	CD	GLU	389	13.894	32.754	-3.632	1.00 50.35
MOTA	2975	0E1		389	13.850	32.799	-4.891	1.00 51.00
MOTA	2976	OE2	GLU	389	12.900	32.464	-2.912	1.00 50.86
MOTA	2977	С	GLU	389	16.476	30.713	-1.635	1.00 43.77
ATOM	2978	0	GLU	389	16.325	29.726	-2.355	1.00 43.53
MOTA	2979	N	SER	390	17.671	31.227	-1.335	1.00 43.84
ATOM	2980	CA	SER	390	18.925	30.697	-1.878	1.00 43.61
ATOM	2981	CB	SER	390	20.112	31.549	-1.425	1.00 43.41
MOTA	2982	OG	SER	390	20.229	32.703	-2.241	1.00 43.45
ATOM	2983	С	SER	390	19.243	29.234	-1.607	1.00 43.62
ATOM	2984	0	SER	390	20.126	28.671	-2.251	1.00 44.11
ATOM	2985	N	ARG	391	18.555	28.614	-0.660	1.00 43.22
MOTA	2986	CA	ARG	391	18.815	27.213	-0.396	1.00 43.67
ATOM	2987	CB	ARG	391	19.174	26.994	1.078	1.00 42.72
ATOM	2988	CG	ARG	391	20.440	27.699	1.512	1.00 41.51
MOTA	2989	CD	ARG	391	20.907	27.245	2892	1.00 39.51
ATOM	2990	NΞ	ARG	391	22.183	27.864	3.231	1.00 37.99
ATOM	2991	CZ	ARG	391	22.940	27512	4.266	1.00 37.81
ATOM	2992	NH1		391	22.545	26.540	5.070	1.00 36.05
ATOM	2993	NH2		391	24.105	28.121	4.482	1.00 37.12
ATOM	2994	С	ARG	391	17.578	26.404	-0.756	1.00 44.95
ATOM	2995	0	ARG	391	17.458	25.241	-0.372	1.00 45.05
ATOM	2996	N	SER	392	16.666	27.023	-1.502	1.00 46.71
MOTA	2997	CA	SER	392	15.420	26.367	-1.895	1.00 48.25
MOTA	2998	CB	SER	392	15.631	25.468	-3.121	1.00 48.10
ATOM	2999	OG	SER	392	15.610	26.216	-4.326	1.00 48.60
ATOM	3000	C	SER	392	14.880	25.536	-0.737	1.00 49.61
MOTA	3001	0	SER	392	14.601	24.344	-0.882	1.00 49.37
MOTA	3002	N	GLU	393	14.749	26.175	0.420	1.00 51.58
ATOM	3003	CA	GLU	393	14.237	25.510	1.617	1.00 53.54
ATOM	3004	CB	GLU	393	15.085	25.897	2.842	1.00 54.33

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Figur 4

Fi	gur 4							
3.001	2005	00	OT 17	202	16 506	05 655		
ATOM	3005	CG	GLU	393	16.586	25.655	2.701	1.00 54.92
ATOM	3006	CD	GLU	393	17.057	24.420	3.450	1.00 55.87
ATOM	3007	OE1	GLU	393	16.845	24.347	4.683	1.00 55.29
MOTA	3008		GLU	393	17.646	23.523	2.806	1.00 56.69
ATOM	3009	С	GLU	393	12.793	25.961	1.838	1.00 54.20
ATOM	3010	0	GLU	393	12.482	27.151	1.693	1.00 53.70
ATOM	3011	N	ASP	394	11.907	25.026	2.173	1.00 55.42
ATOM	3012	CA	ASP	394	10.519	25.404	2.419	1.00 56.88
ATOM	3013	CB	ASP	394	9.585	24.194	2.400	1.00 58.69
ATOM	3014	CG	ASP	394	8.111	24.602	2.415	1.00 61.23
MOTA	3015		ASP	394	7.691	25.298	3.376	1.00 62.29
ATOM	3016		ASP	394	7.374	24.237	1.466	1.00 62.03
MOTA	3017	¢	ASP	394	10.489	26.041	3.795	1.00 56.57
ATOM	3018	0	ASP	394	10.023	27.164	3.959	1.00 56.22
MOTA	3019	N	VAL	395	10.994	25.298	4.773	1.00 56.79
MOTA	3020	CA	VAL	395	11.085	25.756	6.153	1.00 57.23
ATOM	3021	CB	VAL	395	10.166	24.949	7.093	1.00 57.72
ATOM	3022	CG1	VAL	395	10.444	25.320	8.548	1.00 57.64
ATOM	3023	CG2	VAL	395	8.708	25.221	6.749	1.00 58.46
MOTA	3024	С	VAL	395	12.534	25.538	6.575	1.00 57.01
MOTA	3025	0	VAL	395	12.968	24.407	6.793	1.00 56.90
MOTA	3026	N	MSE	396	13.280	26.626	6.690	1.00 56.80
ATOM	3027	CA	MSE	396	14.682	26.536	7.058	1.00 56.12
ATOM	3028	CB	MSE	396	15.463	27.645	6.375	1.00 57.66
MOTA	3029	CG	MSE	396	16.932	27.623	6.690	1.00 60.51
ATOM	3030	SE	MSE	396	17.716	29.077	6.002	1.00 65.26
MOTA	3031	CE	MSE	396	17.988	28.564	4.293	1.00 64.74
MOTA	3032	С	MSE	396	14.964	26.600	8.545	1.00 54.59
ATOM	3033	0	MSE	396	14.487	27.491	9.245	1.00 54.08
ATOM	3034	N	ARG	397	15.740	25.637	9.025	1.00 53.05
ATOM	3035	CA	ARG	397	16.134	25.613	10.426	1.00 51.13
MOTA	3036	CB	ARG	397	16.226	24.181	10.951	1.00 52.77
ATOM	3037	CG	ARG	397	14.888	23.520	11.244	1.00 55.36
ATOM	3038	CD	ARG	397	15.132	22.079	11.671	1.00 58.69
ATOM	3039	NE	ARG	397	13.985	21.448	12.326	1.00 61.28
ATOM	3040	CZ	ARG	397	14.056	20.294	12.990	1.00 62.10
ATOM ATOM	3041	NH1 NH2		397 397	15.215	19.651	13.078	1.00 62.57
ATOM	3042	C	ARG	397	12.978	19.793	13.583	1.00 62.49
ATOM	3043	0	ARG	397	17.509	26.252	10.397	1.00 48.33
ATOM	3045	N	ILE	398	18.273 17.825	26.029	9.466	1.00 47.77
MOTA	3045	CA	ILE	398	19.120	27.064	11.395	1.00 45.82
MOTA	3047	CB	ILE	398	19.202	28.791	10.293	1.00 43.01
ATOM	3047	CG2		398	18.161	29.864	10.293	1.00 43.25
ATOM	3049	CG1		398	20.594	29.417	10.532	1.00 43.16
ATOM	3050	CD1		398	20.768	30.466	9.206	1.00 44.64
ATOM	3051	C	ILE	398	19.441	28.381	12.717	1.00 40.64
ATOM	3052	0	ILE	398	18.557	28.890	13.404	1.00 40.04
ATOM	3053	N	THR	399	20.722	28.360	13.060	1.00 37.78
ATOM	3054	CA	THR	399	21.185	28.954	14.290	1.00 35.36
ATOM	3055	CB	THR	399	22.052	27.988	15.079	1.00 35.02
ATOM	3056		THR	399	21.280	26.832	15.425	1.00 34.92
ATOM	3057	CG2		399	22.570	28.666	16.345	1.00 34.73
MOTA	3058	C	THR	399	22.001	30.197	13.994	1.00 34.73
MOTA	3059	o	THR	399	22.736	30.254	13.994	1.00 35.10
ATOM	3060	N	VAL	400	21.858	31.184	14.871	1.00 32.96
ATOM	3061	CA	VAL	400	22.539	32.457	14.759	1.00 32.30
ATOM	3062	CB	VAL	400	21.514	33.593	14.592	1.00 31.07
ATOM	3063		VAL	400	22.211	34.934	14.415	1.00 31.76
		501	******	200	22.211	54.554	24.415	1.00 31.70

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Offenlegungstag: 17. Juli 2003

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ATO	M 3064	cca	VAL	400	20 600			
ATO		C	VAL	400	20.628	33.298	13.405	1.00 31.47
ATO		ō	VAL	400	23.336	32.685	16.039	1.00 30.19
ATO		N	GLY	401	22.779	32.640	17.144	1.00 30.96
ATO		CA	GLY		24.641	32.905	15.888	1.00 28.35
				401	25.482	33.150	17.041	1.00 24.47
ATO		C O	GLY	401	25.487	34.641	17.235	1.00 23.04
ATO				401	25.595	35.388	16.260	1.00 20.38
		N	VAL	402	25.367	35.086	18.482	1.00 23.36
ATO		CA	VAL	402	25.338	36.514	18.751	1.00 23.38
ATO		CB	VAL	402	23.927	36.960	19.124	1.00 22.79
ATO:			VAL	402	23.790	38.458	18.909	1.00 22.85
ATO		CG2		402	22.895	36.176	18.320	1.00 22.42
ATO		C	VAL	402	26.252	36.899	19.893	1.00 24.25
ATO		0	VAL ASP	402	26.484	36.098	20.794	1.00 25.20
ATO		N CA	ASP	403 403	26.770	38.124	19.848	1.00 24.83
ATO		CB			27.637	38.649	20.894	1.00 27.11
ATO			ASP	403	29.078	38.212	20.691	1.00 30.98
ATO		CG	ASP	403	30.003	38.739	21.787	1.00 34.48
ATO		0D1		403	29.887	39.938	22.122	1.00 36.02
ATO		OD2		403	30.842	37.960	22.311	1.00 36.05
ATO		C O	ASP ASP	403 403	27.562	40.154	20.763	1.00 27.24
ATO		N	GLY		27.550	40.667	19.645	1.00 29.15
ATO		CA	GLY	404 404	27.519	40.863	21.888	1.00 26.60
ATO		C	GLY	404	27.410 26.750	42.316	21.863	1.00 26.50
ATO		Ö	GLY	404	25.810	42.829	23.137	1.00 27.10
ATO		N	SER	405	27.209	42.193	23.665	1.00 26.90
ATO		CA	SER	405	26.638	43.972 44.496	23.644	1.00 26.72 1.00 27.96
ATO		CB	SER	405	27.409	45.722	25.371	1.00 27.98
ATO		OG	SER	405	27.164	46.828	24.521	1.00 28.04
ATO		c	SER	405	25.168	44.857	24.738	1.00 28.25
ATO	M 3095	0	SER	405	24.341	44.473	25, 573	1.00 27.96
ATO	M 3096	N	VAL	406	24.844	45.591	23.675	1.00 27.79
ATO	м 3097	CA	VAL	406	23.465	45.992	23 445	1.00 28.13
ATO	м 3098	CB	VAL	406	23.281	46.667	22.074	1.00 28.02
ATO	M 3099	CG1	VAL	406	21.814	47.063	21.908	1.00 27.91
ATO		CG2	VAL	406	24.197	47.877	21.940	1.00 25.07
ATO		С	VAL	406	22.535	44.789	23.488	1.00 28.35
ATO		0	VAL	406	21.484	44.826	24.120	1.00 28.48
ATO	M 3103	N	TYR	407	22.934	43.718	22.811	1.00 28.72
ATO		CA	TYR	407	22.130	42.493	22.736	1.00 28.45
ATO		CB	TYR	407	22.613	41.643	21.558	1.00 26.86
ATO		CG	TYR	407	21.831	40.373	21.341	1.00 25.29
ATO			TYR	407	20.700	40.358	20.535	1.00 25.44
ATO		CEL	TYR	407	19.964	39.189	20.346	1.00 25.93
ATO		CD2	TYR	407	22.213	39192	21.955	1.00 24.93
ATO		CE2	TYR	407	21.488	38.021	21.780	1.00 25.18
ATO		CZ	TYR	407	20.362	38.024	20.974	1.00 26.03
ATOI		OH	TYR	407	19.626	36.868	20.822	1.00 25.67
ATO		C	TYR	407	22.175	41.651	24.014	1.00 28.83
ATO		0	TYR	407	21.202	40.988	24.369	1.00 28.62
ATO		N	LYS	408	23.306	41.674	24.705	1.00 29.64
ATO		CA	LYS	408	23.440	40.881	25.916	1.00 30.07
ATO		CB	LYS	408	24.904	40.477	26.118	1.00 30.08
ATO		CG	LYS	408	25.442	39.556	25.030	1.00 30.61
ATO		CD	LYS	408	26.597	38.698	25.529	1.00 30.05
ATO		CE	LYS	408	26.799	37.515	24.601	1.00 30.22
ATO		NZ	LYS	408	27.828	36.573	25.097	1.00 30.20
ATO	M 3122	С	LYS	408	22.940	41.551	27.185	1.00 30.82

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3.0004	2122			400				
MOTA	3123	0	LYS	408	22.327	40.901	28.038	1.00 31.98
MOTA	3124	N	LEU	409	23.176	42.853	27.296	1.00 30.97
ATOM	3125	ÇA	LEU	409	22.823	43.598	28.501	1.00 31.11
ATOM	3126	CB	LEU	409	24.006	44.482	28.875	1.00 30.54
ATOM	3127	CG	LEU	409	25.305	43.700	28.962	1.00 29.31
MOTA	3128	CD1	LEU	409	26.372	44.591	29.597	1.00 29.41
ATOM	3129	CD2	LEU	409	25.067	42.423	29.785	1.00 28.16
ATOM	3130	c	LEU	409	21.548	44.441	28.611	1.00 31.44
ATOM	3131	ō	LEU	409	20.978	44.542	29.708	1.00 31.86
ATOM	3132	N	HIS	410	21.122	45.077	27.519	1.00 31.34
ATOM	3133	ÇA	HIS	410				
ATOM	3134		HIS	410	19.929	45.912	27.572	1.00 30.80
		CB			19.732	46.635	26.247	1.00 30.36
MOTA	3135	CG	HIS	410	18.703	47.717	26.303	1.00 29.89
ATOM	3136		HIS	410	18.815	49.060	26.179	1.00 29.29
MOTA	3137		HIS	410	17.362	47.457	26.508	1.00 30.79
MOTA	3138	CE1		410	16.691	48.595	26.505	1.00 29.88
MOTA	3139	NE2	HIS	410	17.548	49.583	26.309	1.00 30.87
MOTA	3140	С	HIS	410	18.728	45.031	27.900	1.00 31.41
MOTA	3141	0	HIS	410	18.467	44.055	27.207	1.00 31.97
MOTA	3142	N	PRO	411	17.985	45.376	28.969	1.00 31.63
ATOM	3143	CD	PRO	411	18.173	46.690	29.610	1.00 31.32
ATOM	3144	ÇA	PRO	411	16.798	44.708	29.518	1.00 31.33
MOTA	3145	CB	PRO	411	16.111	45.815	30.299	1.00 31.27
ATOM	3146	CG	PRO	411	17.257	46.599	30.822	1.00 32.32
MOTA	3147	c	PRO	411	15.827			
ATOM	3148	0				44.037	28.571	1.00 32.09
		N	PRO	411	15.362	42.920	28.838	1.00 32.76
ATOM	3149		SER	412	15.519	44.684	27.457	1.00 31.73
MOTA	3150	CA	SER	412	14.527	44.094	26.573	1.00 31.92
MOTA	3151	CB	SER	412	13.210	44.834	26.771	1.00 32.51
ATOM	3152	OG	SER	412	13.368	46.200	26.390	1.00 33.27
ATOM	3153	С	SER	412	14.838	44.047	25.082	1.00 31.91
ATOM	3154	0	SER	412	14.039	43.520	24.304	1.00 32.59
MOTA	3155	N	PHE	413	15.974	44.601	24.679	1.00 30.72
ATOM	3156	CA	PHE	413	16.348	44.615	23.271	1.00 30.13
ATOM	3157	CB	PHE	413	17.778	45.105	23.130	1.00 28.18
ATOM	3158	CG	PHE	413	18.213	45.285	21.716	1.00 25.96
ATCM	3159	CD1	PHE	413	18.085	46.522	21.094	1.00 25.70
ATOM	3160	CD2	PHE	413	18.772	44.233	21.015	1.00 24.47
ATOM	3161	CE1		413	18.517	46.711	19.787	1.00 25.13
ATOM	3162	CE2		413	19.208	44.408	19.707	1.00 24.84
ATOM	3163	CZ	PHE	413	19.082	45.652	19.092	1.00 24.48
ATOM	3164	c	PHE	413	16.232	43.228	22.645	1.00 31.20
ATOM	3165	o	PHE	413	15.571	43.228	21.612	1.00 31.20
ATOM	3166	N	LYS	414	16.888	42.268	23275	1.00 31.75
ATOM	3167	CA	LYS	414				
ATOM	3168	CB	LYS	414	16.851	40.906	22.790	1.00 32.75
					17.626	39999	23.755	1.00 33.66
ATOM	3169	CG	LYS	414	17.570	38.526	23.429	1.00 34.45
ATOM	3170	CD	LYS	414	18.732	37.744	24.049	1.00 36.05
ATOM	3171	CE	LYS	414	18.845	37.909	25.558	1.00 35.80
ATOM	3172	NZ	LYS	414	19.972	38.817	25.920	1.00 36.66
ATOM	3173	С	LYS	414	15.412	40.411	22.600	1.00 33.19
ATOM	3174	0	LYS	414	15.054	39.927	21.518	1.00 33.30
ATOM	3175	N	GLU	415	14.577	40.542	23.627	1.00 33.81
ATOM	3176	CA	GLU	415	13.193	40.071	23.513	1.00 34.53
ATOM	3177	CB	GLU	415	12.462	40.251	24.838	1.00 37.65
ATOM	3178	CG	GLU	415	13.062	39.497	26.002	1.00 42.83
ATOM	3179	CD	GLU	415	14.376	40.090	26.520	1.00 45.68
ATOM	3180	OE1		415	14.523	41.339	26.526	1.00 47.31
ATOM	3181	OE2		415	15.245	39.293	26.956	1.00 47.44
	3201	JEZ	CHO	413	13.243	32.233	20.330	1.00 47.44

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MOTA	3182	С	GLU	415				
ATOM	3183	o	GLU	415	12.409	40.776	22.401	1.00 33.23
					11.676	40.137	21.649	1.00 33.06
ATOM	3184	N	ARG	416	12.551	42.092	22.299	1.00 31.77
ATOM	3185	CA	ARG	416	11.841	42.825	21.264	1.00 30.32
MOTA	3186	CB	ARG	416	12.066	44.328	21.427	1.00 31.27
MOTA	3187	CG	ARG	416	11.645	44.875	22.796	1.00 33.92
MOTA	3188	CD	ARG	416	11.783	46.393	22.901	1.00 35.48
ATOM	3189	NE	ARG	416	11.545	46.866	24.267	1.00 38.24
MOTA	3190	CZ	ARG	416	11.982	48.030	24.746	1.00 39.11
MOTA	3191	NH1		416	12.676	48.850	23.967	1.00 39.89
ATOM	3192		ARG	416	11.754	48.365	26.009	1.00 38.52
ATOM	3193	С	ARG	416	12.379	42.354	19.916	1.00 29.08
ATOM	3194	0	ARG	416	11.620	42.159	18.964	1.00 28.85
ATOM	3195	И	PHE	417	13.694	42.144	19.862	1.00 27.59
MOTA	3196	CA	PHE	417	14.377	41.707	18.648	1.00 25.70
ATOM	3197	CB	PHE	417	15.886	41.687	18.890	1.00 23.64
MOTA	3198	CG	PHE	417	16.687	41.310	17.680	1.00 20.59
ATOM	3199	CD1		417	16.910	42.230	16.671	1.00 18.99
ATOM	3200	CD2	PHE	417	17.183	40.018	17.540	1.00 19.41
ATOM	3201	CE1	PHE	417	17.610	41.870	15.540	1.00 19.87
MOTA	3202	CE2	PHE	417	17.884	39.641	16.413	1.00 18.04
ATOM	3203	CZ	PHE	417	18.100	40.563	15.409	1.00 20.04
MOTA	3204	С	PHE	417	13.943	40.342	18.099	1.00 25.74
ATOM	3205	0	PHE	417	13.568	40.225	16.927	1.00 25.24
ATOM	3206	N	HIS	418	14.012	39.301	18.922	1.00 26.11
MOTA	3207	CA	HIS	418	13.612	37.962	18.459	1.00 26.79
ATOM	3208	CB	HIS	418	13.638	36.973	19.615	1.00 28.01
MOTA	3209	CG	HIS	418	14.973	36.854	20.279	1.00 28.81
MOTA	3210	CD2	HIS	418	16.168	37.425	19.989	1.00 29.42
MOTA	3211	ND1	HIS	418	15.182	36.067	21.389	1.00 28.15
MOTA	3212	CE1	HIS	418	16.446	36.157	21.755	1.00 29.43
ATOM	3213	NE2	HIS	418	17.067	36.974	20.924	1.00 29.74
MOTA	3214	C	HIS	418	12.209	37.985	17.876	1.00 26.41
ATOM	3215	0	HIS	418	11.976	37.565	16.733	1.00 26.40
ATOM	3216	N	ALA	419	11.284	38.487	18.688	1.00 25.83
ATOM	3217	CA	ALA	419	9.885	38.603	18.328	1.00 25.05
ATOM	3218	CB	ALA	419	9.182	39.454	19.352	1.00 24.80
ATOM	3219	С	ALA	419	9.731	39.215	16.943	1.00 25.35
MOTA	3220	0	ALA	419	9.146	38.601	16.029	1.00 25.99
ATOM	3221	N	SER	420	10.249	40.425	16.777	1.00 25.26
ATOM	3222	CA	SER	420	10.159	41.078	15.481	1.00 25.31
ATOM	3223	CB	SER	420	10.897	42.405	15.515	1.00 23.85
ATOM	3224	OG	SER	420	10.692	43.089	14.303	1.00 23.43
ATOM	3225	С	SER	420	10.751	40.170	14.391	1.00 26.14
MOTA	3226	0	SER	420	10.145	39.976	13331	1.00 25.95
MOTA	3227	N	VAL	421	11.926	39.602	14.670	1.00 27.34
ATCM	3228	CA	VAL	421	12.602	38.699	13.733	1.00 28.41
MOTA	3229	CB	VAL	421	13.919	38.127	14.346	1.00 27.63
ATOM	3230	CG1	VAL	421	14.479	37.020	13.475	1.00 26.36
ATOM	3231	CG2		421	14.953	39.232	14.469	1.00 28.22
MOTA	3232	С	VAL	421	11.689	37.535	13.325	1.00 29.65
ATOM	3233	0	VAL	421	11.557	37.227	12.130	1.00 28.72
MOTA	3234	N	ARG	422	11.069	36.886	14.310	1.00 30.74
ATOM	3235	CA	ARG	422	10.165	35.775	14.014	1.00 32.79
ATOM	3236	CB	ARG	422	9.419	35.328	15.265	1.00 33.29
MOTA	3237	CG	ARG	422	10.259	35.197	16.512	1.00 34.47
ATOM	3238	CD	ARG	422	11.081	33.927	16.558	1.00 34.54
ATOM	3239	NE	ARG	422	11.862	33.905	17.795	1.00 35.75
MOTA	3240	CZ	ARG	422	12.824	33.028	18.066	1.00 35.45

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ATOM	3241	371.71	ARG	422	12 127	20.005		
					13.127	32.085	17.180	1.00 35.35
MOTA	3242		ARG	422	13.490	33.108	19.215	1.00 33.55
ATOM	3243	С	ARG	422	9.123	36.277	13.019	1.00 33.41
ATOM	3244	0	ARG	422	8.949	35.728	11.929	1.00 33.68
ATOM	3245	N	ARG	423	8.446	37.348	13.417	1.00 34.00
ATOM	3246	CA	ARG	423	7.394	37.946	12.622	1.00 34.13
ATOM	3247	CB	ARG	423	7.022	39.301	13.207	1.00 35.16
MOTA	3248	CG	ARG	423	5.538	39.584	13.202	1.00 36.10
MOTA	3249	CD	ARG	423	5.212	40.831	14.012	1.00 37.57
ATOM	3250	NE	ARG	423	5.482	40.682	15.441	1.00 38.90
MOTA	3251	CZ	ARG	423	6.274	41.503	16.133	1.00 40.51
MOTA	3252	NH1	ARG	423	6.874	42.523	15.513	1.00 41.42
ATOM	3253	NH2	ARG	423	6.461	41.324	17.440	1.00 38.76
ATOM	3254	C	ARG	423	7.754	38.100	11.165	1.00 33.94
ATOM	3255	0	ARG	423	6.919	37.849	10.295	1.00 35.59
ATOM	3256	N	LEU	424	8.993	38.494	10.884	1.00 32.85
ATOM	3257	CA	LEU	424	9.418	38.699	9.497	1.00 31.57
ATOM	3258	CB	LEU	424	10.474	39.788	9.450	1.00 28.75
ATOM	3259	CG	LEU	424	10.030	41.129	10.003	1.00 27.64
ATOM	3260		LEU	424	11.220	42.080	10.066	1.00 26.47
MOTA	3261		LEU	424	8.942	41.686	9.115	1.00 27.23
ATOM	3262	C	LEU	424	9.950	37.479	8.747	1.00 27.23
ATOM	3263	ō	LEU	424	10.232	37.562		
ATOM	3264	N	THR	425	10.232		7.551	1.00 31.15
ATOM	3265	CA	THR	425	10.065	36.343	9.424	1.00 33.88
ATOM	3266	CB	THR	425	11.886	35.153	8.778	1.00 35.30
ATOM	3267	OG1	THR	425	11.886	34.722	9.495	1.00 35.17
ATOM	3268	CG2	THR	425		34.463	10.874	1.00 35.24
ATOM	3269	C	THR	425	12.939	35.817	9.399	1.00 35.16
MOTA	3270		THR	425	9.711	33.923	8.675	1.00 37.00
		0			10.059	32.854	9.182	1.00 37.54
ATOM ATOM	3271 3272	N	PRO	426	8.562	34.040	7.982	1.00 38.04
		CD	PRO	426	8.144	35.123	7.073	1.00 38.49
MOTA	3273	CA	PRO	426	7.663	32.890	7.856	1.00 38.85
ATOM	3274	CB	PRO	426	6.745	33.295	6.700	1.00 38.23
ATOM	3275	CG	PRO	426	6.699	34.772	6.802	1.00 38.07
ATOM	3276	C	PRO	426	8.445	31.615	7.527	1.00 39.83
ATOM	3277	0	PRO	426	9.378	31.641	6.728	1.00 40.28
ATOM	3278	N	SER	427	8.073	30.510	8.158	1.00 40.72
ATOM	3279	CA	SER	427	8.713	29.232	7.892	1.00 41.82
ATOM	3280	CB	SER	427	8.358	28.785	6.474	1.00 42.86
ATOM	3281	OG	SER	427	6.954	28.802	6.287	1.00 44.69
MOTA	3282	С	SER	427	10.234	29.228	8.068	1.00 42.10
ATOM	3283	0	SER	427	10.981	28.899	7.140	1.00 41.85
ATOM	3284	N	CYS	428	10.679	29.586	9.267	1.00 42.60
ATOM	3285	CA	CYS	428	12.096	29.608	9 601	1.00 42.43
ATOM	3286	CB	CYS	428	12.724	30.960	9.258	1.00 42.59
MOTA	3287	SG	CYS	428	12.860	31.327	7.492	1.00 44.02
MOTA	3288	С	CYS	428	12.195	29.381	11.096	1.00 42.45
ATOM	3289	0	CYS	428	11.671	30.169	11.879	1.00 43.76
MOTA	3290	N	GLU	429	12.846	28.296	11.494	1.00 42.34
ATOM	3291	CA	GLU	429	13.014	27.995	12.909	1.00 41.23
ATOM	3292	CB	GLU	429	13.030	26.486	13.146	1.00 42.97
MOTA	3293	CG	GLU	429	11.699	25.796	12.933	1.00 45.48
MOTA	3294	CD	GLU	429	11.847	24.282	12.925	1.00 47.43
ATOM	3295	OE1	GLU	429	12.518	23.756	13.847	1.00 48.77
ATOM	3296	OE2	GLU	429	11.298	23.623	12.005	1.00 48.07
ATOM	3297	C	GLU	429	14.341	28.587	13.346	1.00 39.77
ATOM	3298	0	GLU	429	15.370	27.902	13.352	1.00 39.92
ATOM	3299	N	ILE	430	14.315	29.864	13.708	1.00 38.09
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MOTA	3300	CA	ILE	420				
MOTA	3301	CB	ILE	430	15.514	30.560	14.142	1.00 36.48
ATOM	3302	CG2		430	15.341	32.070	13.998	1.00 35.17
				430	16.659	32.770	14.280	1.00 34.48
MOTA	3303	CG1		430	14.839	32.390	12.589	1.00 35.30
MOTA	3304	CD1		430	14.669	33.866	12.310	1.00 34.88
ATOM	3305	С	ILE	430	15.872	30.254	15.591	1.00 37.06
MOTA	3306	0	ILE	430	15.044	30.399	16.495	1.00 38.13
ATOM	3307	N	THR	431	17.109	29.823	15.808	1.00 36.61
MOTA	3308	CA	THR	431	17.600	29.520	17.146	1.00 36.17
ATOM	3309	CB	THR	431	18.067	28.053	17.240	1.00 36.58
ATOM	3310	OG1		431	16.950	27.180	17.031	1.00 36.34
ATOM	3311	CG2	THR	431	18.692	27.774	18.604	1.00 36.38
ATOM	3312	С	THR	431	18.796	30.441	17.396	1.00 36.13
ATOM	3313	0	THR	431	19.705	30.513	16.569	1.00 36.10
ATOM	3314	N	PHE	432	18.804	31.157	18.514	1.00 35.79
ATOM	3315	CA	PHE	432	19.926	32.054	18.794	1.00 35.93
MOTA	3316	CB	PHE	432	19.443	33.450	19.232	1.00 34.31
ATOM	3317	CG	PHE	432	18.643	34.194	18.188	1.00 32.53
MOTA	3318	CD1	PHE	432	17.271	33.977	18.048	1.00 31.59
ATOM	3319	CD2	PHE	432	19.262	35.124	17.353	1.00 31.00
MOTA	3320		PHE	432	16.527	34.676	17.092	1.00 30.53
ATOM	3321		PHE	432	18.525	35.826	16.395	1.00 30.35
ATOM	3322	CZ	PHE	432	17.154	35.600	16.266	1.00 30.25
ATOM	3323	C	PHE	432	20.767	31.483	19.917	1.00 37.08
ATOM	3324	ō	PHE	432	20.248	30.772	20.779	1.00 37.08
ATOM	3325	N	ILE	433	22.063	31.774	19.906	
ATOM	3326	CA	ILE	433	22.933	31.321		1.00 37.32
ATOM	3327	CB	ILE	433	23.526	29.890	20.983	1.00 38.46
ATOM	3328	CG2		433	22.398	28.863	20.722	1.00 39.06
ATOM	3329	CG1	ILE	433	24.367	29.861	20.624	1.00 38.62
ATOM	3330	CD1		433	25.028		19.449	1.00 39.03
MOTA	3331	C	ILE	433	24.039	28.520	19.227	1.00 38.32
ATOM	3332	ō	ILE	433	24.429	32.358	21.161	1.00 39.33
ATOM	3333	N	GLU	434	24.527	33.034	20.201	1.00 39.15
ATOM	3334	CA	GLU	434	25.559	32.505	22.388	1.00 40.58
ATOM	3335	CB	GLU	434	25.152	33.498	22.669	1.00 42.92
ATOM	3336	CG	GLU	434	23.769	34.312	23.885	1.00 43.91
ATOM	3337	CD	GLU	434	23.769	34.883	23.744	1.00 45.53
ATOM	3338		GLU	434		35.640	24.965	1.00 46.68
ATOM	3339	OE2		434	23.436 22.910	35.072	26.074	1.00 47.18
ATOM	3340	C	GLU	434	26.965	36.802	24.816	1.00 48.77
ATOM	3341	ō	GLU	434	27.206	32.950	22.865	1.00 44.01
ATOM	3342	N	SER	435	27.206	32.058	23.680	1.00 44.48
ATOM	3343	CA	SER	435	29.284	33.518	22.119	1.00 45.00
ATOM	3344	CB	SER	435		33.075	22.167	1.00 46.11
ATOM	3345	OG	SER		30.077	33.779	21057	1.00 46.95
ATOM	3346	C	SER	435	29.839	35.186	21.053	1.00 47.94
ATOM	3347	0	SER	435	29.984	33.274	23.507	1.00 46.36
				435	30.043	34.396	24.022	1.00 46.31
ATOM ATOM	3348	N	GLU	436	30.505	32.180	24.069	1.00 46.22
ATOM	3349	CA	GLU	436	31.248	32.250	25.330	1.00 46.33
	3350	CB	GLU	436	31.322	30.884	26.020	1.00 47.64
ATOM	3351	CG	GLU	436	32.144	30.908	27.317	1.00 50.83
ATOM	3352	CD	GLU	436	32.726	29.541	27.711	1.00 52.03
ATOM	3353	OEl		436	31.951	28.585	27.970	1.00 52.84
ATOM	3354	OE2		436	33.972	29.428	27.765	1.00 52.07
ATOM	3355	C	GLU	436	32.650	32.671	24.912	1.00 45.58
ATOM	3356	0	GLU	436	33.446	31.843	24.463	1.00 45.50
ATOM	3357	N	GLU	437	32.950	33.956	25.051	1.00 44.67
MOTA	3358	CA	GLU	437	34.252	34.462	24.643	1.00 44.13

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ATOM	3359	СВ	GLU	437	35.328	34.050	25 650	1 00 42 61
ATOM	3360	CG	GLU	437	36.745	34.334	25.652	1.00 43.61
ATOM	3361	CD	GLU	437	36.931	35.752	25.190 24.678	1.00 43.39
ATOM	3362	OE1	GLU	437	36.976	36.680		1.00 43.50
ATOM	3363	OE2	GLU	437	37.025	35.940	25.514	
ATOM	3364	C	GLU	437	34.569	33.880	23.441	1.00 42.17
ATOM	3365	ō	GLU	437	35.530	33.131	23.264	1.00 43.56
MOTA	3366	И	GLY	438	33.757	34.225	23.108	1.00 45.30
ATOM	3367	CA	GLY	438	33.958	34.225	22.266	1.00 41.68
ATOM	3368	C	GLY	438	34.748		20.926	1.00 39.44
ATOM	3369	ō	GLY	438	34.748	34.538	19.934	1.00 38.11
ATOM	3370	N	SER	439	35.213	34.130	18.791	1.00 37.45
ATOM	3371	CA	SER	439		35.713	20.329	1.00 37.14
ATOM	3372	CB	SER	439	35.980	36.502	19.386	1.00 36.86
ATOM	3373	OG	SER	439	35.916	37.983	19.714	1.00 36.81
ATOM	3374	C	SER	439	36.825	38.678	18.878	1.00 35.32
ATOM	3375	ō	SER	439	37.420	36.053	19.444	1.00 36.74
ATOM	3376	N	GLY	440	38.192	36.265	18.513	1.00 36.37
ATOM	3377	CA	GLY	440	37.774	35.439	20.562	1.00 36.58
ATOM	3378	C	GLY	440	39.126 39.207	34.957	20.746	1.00 36.42
ATOM	3379	ō	GLY	440		33.518	20.302	1.00 36.28
ATOM	3380	N	ARG	441	40.146	33.140	19.613	1.00 36.20
ATOM	3381	CA	ARG	441	38.224	32.714	20.699	1.00 36.09
ATOM	3382	CB		441	38.190	31.309	20.312	1.00 37.16
ATOM	3383	CG	ARG ARG	441	37.151	30.562	21.138	1.00 37.34
ATOM	3384	CD	ARG	441	37.312	30.717	22.632	1.00 39.57
ATOM	3385	NE	ARG	441	36.334	29.806	23.375	1.00 42.28
ATOM	3386	CZ	ARG	441	35.270	29.339	22.488	1.00 44.36
ATOM	3387	NH1	ARG	441	34.240	28.585	22.862	1.00 45.80
ATOM	3388	NH2	ARG	441	34.103	28.192	24.127	1.00 45.87
ATOM	3389	C	ARG	441	37.848	28.214	21.955	1.00 47.26
ATOM	3390	ō	ARG	441	38.103	31.179	18.821	1.00 37.42
ATOM	3391	N	GLY	442	37.270	30.151	18.189 18.262	1.00 37.52 1.00 37.34
ATOM	3392	CA	GLY	442	36.906	32.234	16.863	1.00 37.34
ATOM	3393	C	GLY	442	38.165	32.308	16.048	1.00 37.39
ATOM	3394	ō	GLY	442	38.483	31.410	15.278	1.00 37.47
ATOM	3395	N	ALA	443	38.887	33.408	16.241	1.00 37.31
ATOM	3396	CA	ALA	443	40.134	33.660	15.526	1.00 38.50
ATOM	3397	CB	ALA	443	40.739	34.999	15.967	1.00 36.50
ATOM	3398	C	ALA	443	41.127	32.521	15.759	1.00 39.03
ATOM	3399	0	ALA	443	42.015	32.297	14.941	1.00 39.36
ATOM	3400	N	ALA	444	40.977	31.807	16.875	1.00 39.93
ATOM	3401	CA	ALA	444	41.864	30.685	17.172	1.00 40.31
ATOM	3402	CB	ALA	444	41.724	30.242	18.623	1.00 39.25
ATOM	3403	C	ALA	444	41.427	29.569	16246	1.00 40.97
ATOM	3404	0	ALA	444	42.146	29210	15.312	1.00 41.31
ATOM	3405	N	LEU	445	40.233	29.038	16.501	1.00 41.41
ATOM	3406	CA	LEU	445	39.678	27.960	15.690	1.00 41.97
ATOM	3407	CB	LEU	445	38.195	27.776	16.024	1.00 40.09
ATOM	3408	CG	LEU	445	37.954	26.806	17.182	1.00 39.14
MOTA	3409	CD1		445	36.750	27.233	17.982	1.00 39.27
ATOM	3410	CD2		445	37.781	25.399	16.647	1.00 37.36
MOTA	3411	C	LEU	445	39.860	28.156	14.176	1.00 43.29
ATOM	3412	0	LEU	445	39.918	27.179	13.427	1.00 43.28
ATOM	3413	N	VAL	446	39.955	29.406	13.729	1.00 44.66
MOTA	3414	CA	VAL	446	40.136	29.684	12.307	1.00 46.32
ATOM	3415	CB	VAL	446	39.687	31.120	11.948	1.00 46.15
ATOM	3416	CG1		446	40.356	31.578	10.653	1.00 46.15
ATOM	3417	CG2	VAL	446	38.164	31.160	11.793	1.00 45.75

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ATOM	3418	С	VAL	446	41 500			
ATOM	3419	ō	VAL	446	41.597	29.503	11.944	1.00 48.03
ATOM	3420	N	SER	447	41.929	29.105	10.825	1.00 48.75
ATOM	3421	CA	SER	447	42.465	29.802	12.904	1.00 49.63
ATOM	3422	CB	SER	447	43.902	29.657	12.725	1.00 50.76
ATOM	3423	OG	SER		44.635	30.267	13.918	1.00 50.76
ATOM	3424	C	SER	447	44.377	31.659	14.021	1.00 50.83
ATOM	3425	0		447	44.259	28.173	12.612	1.00 52.07
ATOM	3425		SER	447	44.923	27.753	11.662	1.00 52.17
ATOM	3427	N CA	ALA	448	43.804	27.387	13.584	1.00 53.51
ATOM	3428	CB	ALA	448	44.071	25.953	13.621	1.00 55.46
ATOM	3428		ALA	448	43.273	25.306	14.745	1.00 55.02
ATOM	3430	C	ALA	448	43.751	25.263	12.300	1.00 57.02
ATOM	3430	0	ALA	448	44.599	24.564	11.726	1.00 57.18
ATOM		N	VAL	449	42.523	25.457	11.825	1.00 58.39
ATOM	3432 3433	CA	VAL	449	42.093	24.841	10.579	1.00 59.69
MOTA		CB	VAL	449	40.571	24.977	10.382	1.00 59.67
MOTA	3434 3435		VAL	449	40.152	24.262	9.112	1.00 60.28
		CG2		449	39.833	24.384	11.577	1.00 59.48
ATOM ATOM	3436	C	VAL	449	42.821	25.482	9.403	1.00 60.70
ATOM	3437	0	VAL	449	42.903	24.898	8.321	1.00 61.00
ATOM	3438 3439	N	ALA	450	43.361	26.677	9.627	1.00 61.41
ATOM	3440	CA	ALA	450	44.093	27.392	8.591	1.00 62.12
ATOM		CB		450	43.981	28.889	8.814	1.00 62.32
MOTA	3441 3442	C	ALA	450	45.558	26.973	8.606	1.00 63.02
MOTA	3443	O N	ALA	450	46.437	27.748	8.217	1.00 62.75
ATOM	3444	CA	CYS	451	45.807	25.744	9.061	1.00 64.03
MOTA	3445	CB	CYS	451 451	47.160	25.183	9.148	1.00 65.19
ATOM	3446	SG	CYS	451	47.530	24.440	7.850	1.00 65.75
ATOM	3447	C	CYS	451	46.901	22.720	7.723	1.00 66.86
ATOM	3448	ō	CYS	451	48.239	26.217	9.474	1.00 65.22
ATOM	3449		CYS	451	47.929	27.230	10.144	1.00 65.18
ATOM	3450	C1	HEX	1	49.398 31.023	25.979	9.073	1.00 65.50
ATOM	3451	C2	HEX	1		47.521	12.611	1.00 25.83
ATOM	3452	C3	HEX	1	32.239	47.182	11.801	1.00 25.25
ATOM	3453	C4	HEX	1	32.203	45.697	11.565	1.00 25.11
MOTA	3454	C5	HEX	1	31.030	44.939	12.862	1.00 24.99
ATOM	3455	C6	HEX	î	30.772	44.921	13.785	1.00 25.34
ATOM	3456	01	HEX	î	30.750	48.942	15.126 12.579	1.00 25.58
ATOM	3457	02	HEX	1	32.183	47.912	10.609	1.00 27.04
ATOM	3458	03	HEX	í	33.337	45.251	10.836	1.00 25.99
ATOM	3459	04	HEX	1	31.699	43.621	12.545	1.00 25.85
ATOM	3460	05	HEX	1	31.267	46.968	13.935	1.00 25.37
ATOM	3461	06	HEX	1	31.835	45.222	16.009	1.00 27.23
ATOM	3462	Cl	LIG	1	30.034	26.620	8.669	1.00 27.23
ATOM	3463	C2	LIG	1	29.909	27.259	10.064	1.00 34.82
ATOM	3464	C3	LIG	1	31.308	27.852	10.344	1.00 35.54
ATOM	3465	C4	LIG	1	32.212	27.447	9.148	1.00 35.52
ATOM	3466	C5	LIG	.1	31.520	26.207	8.584	1.00 35.20
ATOM	3467	C6	LIG	1	33.670	27.245	9.637	1.00 36.33
ATOM	3468	C7	LIG	1	34.562	25.321	8.758	1.00 37.11
ATOM	3469	C8	LIG	1	35.946	26.832	8.778	1.00 36.91
MOTA	3470	N9	LIG	1	36.382	27.317	7.570	1.00 36.92
MOTA	3471	C10		1	37.668	27.907	7.331	1.00 36.42
ATOM	3472	N11		1	38.035	28.336	6.087	1.00 37.39
ATOM	3473	C12		1	39.058	28.930	6.462	1.00 36.99
ATOM	3474		LIG	1	39.426	29.003	7.575	1.00 37.10
ATOM	3475	S14		1	38.681	28.342	8.700	1.00 37.86
ATOM	3476	015	LIG	1	36.640	26.843	9.817	1.00 38.32

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ATOM 3477 C16 LTG 1 34.538 24.890	9,296 1.00 37.59
ATOM 3478 C17 LIG 1 34.906 24.620	10.610 1.00 37.22
34.030 23.340	11.130 1.00 38.09
1 34.004 22.371	10.404 1.00 38.80
33.723 22.398	9.128 1.00 38.90
ATOM 3482 C21 LIG 1 33.942 23.860	8.546 1.00 38.73
ATOM 3483 K1 K 1 32.471 32.037	-7.104 1.00 46.91
END	7.104 1.00 40.51